Ψ_k Newsletter

AB INITIO (FROM ELECTRONIC STRUCTURE) CALCULATION OF COMPLEX PROCESSES IN MATERIALS

Number 41 October 2000

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Contents

1 Editorial

Since it is the first Psi-k Newsletter after the Psi-k 2000 Conference, in the **General News** section we give some conference statistics, including the final programme and the concluding remarks by Volker Heine. In the **TMR1** section there are two announcements of interesting workshops, and the **RTN** section contains announcements of a few post-doctoral positions and a summer school in Prague next year. In the **TMR2** section readers will find a mid-term review of this network, which includes also some scientific highlights. In the **ESF** section we have three reports on conference/workshops, two of them contain also abstracts of presented talks and posters. Abstracts of newly submitted papers are placed in the usual **Abstracts** section. General position announcements, namely those not linked to any of the networks, can be found in the General Job Announcements section. The newsletter is finished with the scientific highlight of the month by *D. Hobbs, G. Kresse, and J. Hafner* on **"Fully unconstrained noncollinear magnetism within the PAW method"**. Please see the table of contents for further details.

The *Networks* have a home page on World Wide Web (WWW). Its *Uniform Resour ce Locator* (URL) is:

http://psi-k.dl.ac.uk/

The above contains pointers to home pages of some of the members of our electronic structure community. If you maintain a home page on your activities we will be happy to include a pointer from the *Networks'* home page to your home page.

Please note that the home page of the Psi-k Networks has recently been updated. It contains useful information regarding funding of workshops and collaborative visits within the ESF Programme. Its major new feature is a separate highlight section which contains all highlight articles of the Newsletters published so far.

Please submit all material for the next newsletters to the email address below.

The following email addresses, which remain in operation, are repeated for your convenience, and are the easiest way to contact us.

	function
psik-coord@daresbury.ac.uk	**messages to the coordinators, editor & newsletter**
psik-management@daresbury.ac.uk	**messages to the NMB of all Networks**
psik-network@daresbury.ac.uk	**messages to the whole Ψ_k community**

Dzidka Szotek and Walter Temmerman
e-mail: psik-coord@dl.ac.uk

2 General News

2.1 Report on Psi-k2000 Conference

Schwäbisch Gmünd, 22-26 August, 2000

"Ab Initio (from electronic structure) calculations of complex proceses in materials"

This report we start with some statistics regarding the Psi-k 2000 Conference, followed by the conference programme, as it was implemented in reality, and finish with the concluding remarks by Volker Heine.

The conference was run in three parallel sessions over four days, August 23-26, 2000. There were 4 plenary talks, 101 invited talks, 112 contributed talks, and about 160 posters. For the latter there were two dedicated four-hour long evening sessions, where free food and drinks were also available to keep participants relaxed and motivated till late hours. There were some last minute panics and cancellations, but as can be seen from the attached programme, nearly all talks went as planned.

The conference was attended by 424 participants. Among the European countries, the largest amount of participants was from Germany (137), the next was Great Britain (53), then France (29), Austria (22), Italy (20), Finland (19), Sweden (19), Spain (13), The Netherlands (10), Denmark (9), Czech Republic (8), Poland (5), Switzerland (5), Ireland (4), Belgium (3), Russia (3), Greece (2), Hungary (2), Portugal (2), Norway (1), Slovakia (1), Slovenia (1), and Ukraine (1). From outside Europe, we had 31 participants from the USA, 15 from Japan, 3 from Brazil, 3 from India, 2 from Argentina, and 1 from New Zealand.

We would like to take this opportunity and thank once more all the participants for contributing papers, and for making the conference such a lively event.

Psi-k 2000 Conference Programme

Tuesday, 22 August 2000

15:00–20:00 Registration

Wednesday, 23 August 2000

08:00–08:35 Registration

Wednesday Morning Session, Parler room: Opening and Plenary
Chair: R.M. Nieminen

08:40–08:55 Welcome

09:00–09:50 M. Scheffler
The cutting edge: Surfaces and their role in materials' properties

Wednesday Morning Session, Baldung room: CORR-SYS
Chair: B.L. Gyorffy

10:00–10:30 W.E. Pickett, A. B. Shick, R. Weht
Coexistence of high temperature superconductivity and magnetism: $RuSr_2GdCu_2O_8$

10:30–11:00 Coffee

11:00–11:30 Antoine Georges
Introduction to dynamical mean field theory and prospects for electronic structure calculations of correlated materials

11:30–11:45 M. Fleck, E. Pavarini, and O. K. Andersen
Electronic Structure of the striped phase in $La_{2-x-y}Nd_ySr_xCuO_4$

11:45–12:00 V. Drchal, J. Kudrnovský, and V. Janiš
Dynamical electron correlations in transition metals and their alloys

12:00–12:15 K. Terakura, Z. Fang, K. Miura, J. Kanamori
Ferromagnetism and antiferromagnetism in double perovskites: La_2FeCrO_6, Sr_2FeMoO_6 and Sr_2FeWO_6

12:15–12:30 Takeo Fujiwara, Michael Korotin, and Vladimir Anisimov
Long period orbital order with hole stripes in $La_{7/8}Sr_{1/8}MnO_3$

Wednesday Morning Session, Parler room: SEMIC
Chair: R.M. Nieminen

10:00–10:30 Coffee

10:30–11:00 M. Hierlemann
Quantum chemical calculation in an industrial environment

11:00–11:30 U. Lindenfelt
Electronic structure of intrinsic and doped SiC

11:30–11:45 M. Bockstedte, A. Mattausch, and O. Pankratov
Boron diffusion in SiC: the role of intrinsic point defects

11:45–12:00 J. Pollmann, P. Krüger, W. Lu, and M. Rohlfing
Theory of structural and electronic properties of SiC surfaces

12:00–12:30 P. Blöchl
Hydrogen electrochemistry in SiO_2 related to breakdown of gate oxides

Wednesday Morning Session, Ratgeb room: POLYM
Chair: M. Springborg

10:00–10:30 H. Weiss, M. Boero, and M. Parrinello
DFT as a versatile tool in industrial catalysis research

10:30–10:45 J.-W. van der Horst, P.A. Bobbert, M.A.J. Michels, G. Brocks, P.J. Kelly
Electronic and optical properties of conjugated polymers from first principles

10:45–11:00 C. Katan, P. Rabiller, M. Souhassou
Charge density analysis in molecular charge transfer complexes: a comparison between experiment and PAW calculations

11:00–11:30 Coffee

11:30–12:00 M. Côté, Peter D. Haynes, and Carla Molteni
New polymers for optoelectronic applications

12:00–12:30 I. Frank
Chemical reactions induced by mechanical stress: ab-initio simulation

12:30–14:00 Lunch

Wednesday Afternoon Session, Baldung room: MATER
Chair: J.L. Martins

14:00–14:15 Rossitza Pentcheva, Matthias Scheffler, and Kirsten Fichthorn
Influence of substitutional adsorption on the initial growth of Co on Cu(001): a DFT-kMC study

14:15–14:30 B. Winkler, C. J. Pickard, V. Milman, G. Thimm
Systematic prediction of crystal structures and its application to sp^2-carbon polymorphs

14:30–15:00 G. Bihlmayer, Ph. Kurz, F. Förster, and S. Blügel
The FLAPW method applied to complex magnetic systems

15:00–15:30 Kristen A. Fichthorn
Island nucleation in thin-film epitaxy: a multi-scale study

15:30–16:00 Zhong Fang
Applications of ultrasoft pseudopotentials to 3d and 4d transition metal oxides

16:00–16:30 Coffee

Wednesday Afternoon Session, Parler room: SURF
Chair: J. Hafner

14:00–14:30 Catherine Stampfl
Ab initio modelling of temperature-programmed desorption of molecules from metallic surfaces

14:30–14:45 A. Groß, A. Eichler, J. Hafner, F. Kirchhoff, M.J. Mehl, and D.A. Papaconstantopoulos
Ab initio derived tight-binding molecular dynamics simulation of O_2/Pt(111): new unified picture of the molecular adsorption process

14:45–15:00 M.V. Ganduglia-Pirovano, K. Reuter, M. Scheffler
Surface core-level shifts as a probe of the local overlayer structure: O on Rh(111) and Ru(0001)–a DFT study

15:00–15:15 D. Ceresoli, M. Bernasconi, S. Iarlori, M. Parrinello, E. Tosatti
Two-membered silicon rings on a dehydroxylated surface of silica

15:15–15:30 T. T. Rantala,T. S. Rantala, and V. Lantto
Surface relaxation and electronic structure of SnO_2 (110) surface

15:30–16:00 Alexander Bogicevic
Atomistic concepts in epitaxial growth

16:00–16:30 Coffee

Wednesday Afternoon Session, Ratgeb room: BSM
Chair: R. Zeller

14:00–14:30 O.K. Andersen and T. Saha-Dasgupta
Muffin tin orbitals of arbitrary order (NMTOs)

14:30–15:00 T. Saha-Dasgupta and O. K. Andersen
Tight-binding modeling and generation of first-principles Wannier-like orbitals using the new NMTO scheme

15:00–15:30 L. Vitos, H. L. Skriver, and J. Kollar
Application of the exact muffin-tin orbitals theory

15:30–15:45 Helmut Eschrig, Klaus Koepernik
Density functional theory of low temperature phase diagrams: magnetism in the $[Fe(Mn)]_{(1-x)}Al_x$ system

15:45–16:00 Elisabeth Sjöstedt and Lars Nordström
A cautious linearization of the full-potential APW method

16:00–16:30 Coffee

Wednesday Late Afternoon Session, Baldung room: NANO/QD
Chair: A. Rubio

16:30–16:45 S. Siljamäki, R.M. Nieminen, A. Harju
Various spin-polarization states of a quantum dot in high magnetic field: a quantum Monte Carlo study

16:45–17:00 T. Torsti, M. Heiskanen, M.J. Puska, and R.M. Nieminen
Calulations of multiple excitons in InAs quantum dots

17:00–17:15 J. M. Pacheco, José Luís Martins
First principles Monte-Carlo optimization of geometries of large alkali clusters

17:15–17:30

17:30–18:00 T. N. Todorov, A. P. Sutton, and J. Hoekstra
Current-induced mechanical effects in atomic-scale conductors

18:00–18:30 D. Sánchez-Portal, E. Artacho, J. Junquera, J. M. Soler
P. Ordejón, A. García
Monatomic gold wires

18:30–19:00 Marco Buongiorno Nardelli
Theory of electronic and transport properties of carbon nanotubes

Wednesday Late Afternoon Session, Parler room: SURF
Chair: A. Kiejna

16:30–16:45 Andrei Ruban
Local equilibria in Fe/Ru(0001)

16:45–17:00 J. Gottschalck and B. Hammer
The adsorption of S and SH at Au(111)

17:00–17:30 Ali Alavi
Chemistry at metal surfaces from density-functional theory

17:30–17:45 Jose M. Soler, Emilio Artacho, and Gabriel Fabricius
Structure of the liquid silicon surface

17:45–18:00 J. Neugebauer, T. K. Zywietz, M. Scheffler, J. E. Northrup
Adatom kinetics on and below the surface: The presence of a novel diffusion channel

18:00–18:30 Alessio Filippetti and Vincenzo Fiorentini
Theory and applications of the stress density

18:30–19:00 Yoshitada Morikawa and Kiyoyuki Terakura
Ab initio study of methanol synthesis over Zn-deposited Cu surfaces

Wednesday Late Afternoon Session, Ratgeb room: BSM
Chair: G.M. Stocks

16:30–17:00 P. H. Dederichs, N. Papanikolaou, and R. Zeller
Conceptional improvements of the KKR method

17:00–17:30 Nicola Marzari and David Vanderbilt
Localized Wannier functions in extended systems: theory and applications

17:30–18:00 E. E. Krasovskii and W. Schattke
Electronic structure of bulk and semi-infinite crystals by the extended LAPW-kp method

18:00–18:15 A. Mavromaras, A. Ponceau, I. Lado Touriño, F. Tsobnang,
J. Sticht, and E. Wimmer
Optimized basis sets in a full potential LMTO method

18:15–18:30 Marek Hytha, Jiří Vackář and Antonin Šimůnek
Core-level shifts within pseudopotential framework

18:30–18:45 Antonín Šimůnek and Jiří Vackář
Semicore states in all electron pseudopotentials: ground state properties of NaCl

18:45–19:00 G. Theurich, N. A. Hill
General local spin density approximation for plane wave pseudopotential calculations

Wednesday Evening Session

19:00–23:00 Food and Posters

Thursday, 24 August 2000

Thursday Morning Session, Parler room: Plenary
Chair: B. Johansson

08:30–09:25 N. Lang
DFT studies in molecular electronics

Thursday Morning Session, Baldung room: MATER
Chair: M. Gillan

09:30–10:00 R. Martoňák, C. Molteni, L. Colombo, M. Parrinello
Molecular dynamics with a classical pressure reservoir: simulation of pressure-induced transformations in silicon clusters

10:00–10:30 Luciano Colombo
Science-based engineering of defects in silicon by tight-binding molecular dynamics DFT studies in molecular electronics

10:30–11:00 Coffee

11:00–11:15 Rubén Pérez, Peter Gumbsch
Directional anisotropy in the cleavage fracture of silicon

11:15–11:30 W.Mannstadt, A.Canning, A.J. Freeman
Large scale computing and complex materials with the massive parallel FLAPW method

11:30–12:00 G. Kresse
Fast all-electron ab-initio molecular dynamics

12:00–12:15 M. Ikeda, G. Kresse, and J. Hafner
First principles study of bi-layered ferroelectric perovskite materials

12:15–12:30 Na Sai, B. Meyer, and David Vanderbilt
Design of novel ferroelectric materials via compositional inversion symmetry breaking

Thursday Morning Session, Parler room: MAGNET
Chair: B. Johansson

09:30–10:00 I. A. Abrikosov, B. Johansson, Mark van Schilfgaarde
Understanding the INVAR effect in Fe-Ni alloys

10:00–10:30 Coffee

10:30–11:00 J.B. Staunton, J. Poulter, B. Ginatempo, E. Bruno, D.D. Johnson
Spin fluctuations in nearly magnetic metals from ab-initio dynamical spin susceptibility calculations

11:00–11:30 László Udvardi, László Szunyogh, Peter Weinberger
Ab–initio determination of the width of Bloch–wall in Fe

11:30–11:45 H. Ebert, M. Deng, and H. Freyer
Relativistic calculation of magnetic linear response functions using the KKR-Green's function method

11:45–12:00 J. Zabloudil, R. Hammerling, P. Weinberger, C. Uiberacker
Magnetic anisotropy of Co on Cu(111) including relaxation effects

12:00–12:15 Sonia Frota-Pessôa
Exchange coupling from first principles in nonperiodic systems

12:15–12:30 J. Enkovaara, A. Ayuela, R.M. Nieminen, L. Nordström
Magnetic and orbital anisotropy in Ni_2MnGa from first principles

Thursday Morning Session, Ratgeb room: INTERF
Chair: M. Finnis

09:30–10:00 S. Köstlmeier and C. Elsässer
Ab-initio investigation of metal/ceramic bonding: metal/spinel interfaces

10:00–10:15 C. Elsässer, S. Nufer, A. G. Marinopoulos, T. Gemming, W. Kurtz, S. Köstlmeier, and M. Rühle
Microscopic analysis of the rhombohedral twin grain boundary in alumina

10:15–10:30 Kurt Scheerschmidt and Detlef Conrad
Modified empirical potentials for molecular dynamics modelling of bonded interfaces

10:30–11:00 Alfredo Pasquarello
Atomic structure at the interface between silicon and its oxide

11:00–11:30 Coffee

11:30–11:45 Philip Lindan
Interfaces between oxides and aqueous solutions

11:45–12:00 Masanori Kohyama
Strength and fracture of SiC grain boundaries: Ab Initio tensile tests

12:00–12:30 Wielfried Sigle
Electron microscopy studies of grain boundary and interface structures

12:30–14:00 Lunch

Thursday Afternoon Session, Baldung room: CORR-SYS
Chair: K. Terakura

14:00–14:15 P.Blaha, K.Schwarz, P.Novak
Charge distribution and EFGs in cuprates using LDA+U within the LAPW method

14:15–14:30 R. Tyer, W.M.Temmerman, Z. Szotek, H. Winter, and G.A.Gehring
Application of the self-interaction correction to $LaMnO_3$ and $CaMnO_3$

14:30–15:00 I. V. Solovyev
Aspects of charge, spin, and orbital ordering in manganites

15:00–15:30 A. Lichtenstein
Electronic structure of correlated systems: beyond LDA

15:30–15:45 Franca Manghi, Stefano Monastra, Catia Arcangeli
On-site correlation in the photoemission of transition metals

15:45–16:00 C.H. Patterson and M. Nicastro
Exchange coupling in manganites and cuprates

16:00–16:30 Coffee

Thursday Afternoon Session, Parler room: SURF
Chair: E. Wimmer

14:00–14:30 J. Nørskov
Catalysis from first principles?

14:30–15:00 Hervé Toulhoat and Pascal Raybaud
Periodic trends and synergy effects in hydrodesulfurization catalysts: recent findings based on electronic structure calculations

15:00–15:15 Sönke Lorenz, Matthias Scheffler, Axel Groß
Reactions on surfaces with neural networks

15:15–15:30 R. Heid and K.-P. Bohnen
First principles investigations of the lattice dynamics of the Ru(0001) and O(1×1)/Ru(0001) surfaces

15:30–16:00 J. Kollár, L. Vitos, B. Johansson, H. L. Skriver
Stability of surfaces and small particles; surface, step, and kink formation energies

16:00–16:30 Coffee

Thursday Afternoon Session, Ratgeb: SPECTR
Chair: H. Ebert

14:00–14:30 Josef Redinger
First-principles simulation of scanning tunneling microscopy and spectroscopy

14:30–14:45 F. Máca, W.A. Hofer, J. Redinger
Comparison between ab-initio simulation and STM-images for Co/Pt(110) surfaces

14:45–15:00 M. Woods, P. Strange, A. Ernst, and W. M. Temmerman
Relativistic theory of photoemission from magnetic surfaces

15:00–15:30 A T Paxton
Near edge structure in energy-loss spectroscopy of transition metal nitrides: some many electron and magnetic effects using density functional theory

15:30–16:00 N. Lorente and M. Persson
First principles calculations of single molecule vibrational spectroscopy and microscopy

16:00–16:30 Coffee

Thursday Late Afternoon Session, Baldung room: MAGNET
Chair: J. Kübler

16:30–16:45 K. Schwarz, G. K. H. Madsen, and P. Blaha
Unusual magnetism in sodium or potassium electro sodalite (SES or PES)

16:45–17:00 I. Turek
Exchange interactions in itinerant magnets

17:00–17:30 Mark R. Pederson
Molecular magnets: anisotropy energies and resonant tunneling fields within DFT

17:30–18:00 S. Blügel, X. Nie, and G. Bihlmayer
Magnetic anisotropy in low dimensional systems

18:00–18:15 S. Heinze, Ph. Kurz, G. Bihlmayer, D. Wortmann, X. Nie, S. Blügel, M. Bode, A. Kubetzka, O. Pietzsch, R. Wiesendanger
Resolving complex atomic-scale spin-structures by spin-polarized STM

18:15–18:30 V. Ledentu, D. Spisak, J. Hafner
Structure and magnetism of Fe/Ge multilayers

18:30–19:00 Stefano Baroni
Magnons in real materials from density functional theory

Thursday Late Afternoon Session, Parler room: SEMIC
Chair: P. Kratzer

16:30–17:00 J. Ortega, R. Pérez, and F. Flores
Electron correlation effects and dynamical fluctuations at semiconductor surfaces: Sn/Si(111) and Sn/Ge(111)

17:00–17:15 P. Alippi, L. Colombo, A. Sieck, G. Seifert, T. Frauenheim
Boron related defects in silicon by density functional based tight-binding simulations

17:15–17:30 M. Hakala, M. J. Puska, and R. M. Nieminen
First-principles calculations of interstitial B in Si

17:30–17:45 G. Brocks, J.H. Snoeier, P. J. Kelly, E. Zoethout, H. J. W. Zandvliet, and B. Poelseman
The initial stages of growth on the Ge(001) surface: a joint theoretical and experimental study

17:45–18:00 G. Schwarz, J. Neugebauer, and M. Scheffler
Point defects in supercells: convergence with respect to cell size and charge compensation

18:00–18.30 Kurt Schroeder, Armin Antons, Ralf Berger, Stefan Blügel
Theory of surfactant-mediated growth

18:30–18:45 K. Seifert-Lorenz, J. Hafner, G. Kresse
Ab-initio MD of liquid Te and telluriumrich K-Te alloys

18:45–19:00 Fabio Bernardini and Vincenzo Fiorentini
Non-linear behavior of spontaneous polarization in III-V nitrides alloys

Thursday Late Afternoon Session, Ratgeb room: LARGE-SYS
Chair: J. M. Soler

16:30–17:00 D.G. Pettifor, I.I. Oleinik, and D. Nguyen-Manh
Bond-order potentials: bridging the electronic to atomistic modelling hierarchies

17:00–17:15 Takeo Hoshi and Takeo Fujiwara
Theory of Wannier states and order-N electronic structure calculations

17:15–17:30 A. Canning, W. Mannstadt, Wen-tong Geng, and A.J. Freeman
Parallelization of the FLAPW method and applications to large systems

17:30–18:00 Pablo Ordejón
Numerical-atomic-orbitals DFT approach for large systems: applications of SIESTA

18:00–18:30 Stefan Goedecker
Linear scaling methods for electronic structure calculations

18:30–19:00 D.R. Bowler, T.Miyazaki, and M.J.Gillan
Conquest: principles and applications of a linear scaling DFT code

Thursday Evening Session

19:00–23:00 Food and Posters

Friday, 25 August 2000

Friday Morning Session, Parler room: Plenary
Chair: K. Schwarz

08:30–09:25 E.K.U. Gross
New directions in density functional theory

Friday Morning Session, Baldung room: SPECTR
Chair: P. Strange

09:30–10:00 I. Galanakis, M. Alouani, H. Dreyssé
Calculated X-ray magnetic circular dichroism of binary alloys and surfaces
10:00–10:30 Coffee
10:30–11:00 Krister Karlsson, O. Gunnarsson, and O. Jepsen
Cuprate core-level line shapes for different Cu-O networks
11:00–11:30 Gerrit van der Laan
Configuration interaction effects in core-level dichroism of magnetic materials
11:30–11:45 Walter R. L. Lambrecht and Sergey N. Rashkeev
Nonlinear optical response calculations in chalcopyrite semiconductors and the relation to their band structures
11:45–12:00 Jeroen van den Brink, Eva Pavarini, Patrizia Benedetti, Assunta Vigliante, Peter Wochner
Ab initio calculation of resonant X-ray scattering in manganites
12:00–12:30 S. Crampin, E. Arola, M. James, L. Calmels, J.E. Inglesfield
Calculation of second harmonic generation from magnetic interfaces

Friday Morning Session, Parler room: DFT
Chair: K. Schwarz

09:30–10:00 Raffaele Resta
Macroscopic polarisation and electron localisation in extended systems

10:00–10:15 P. García-González, P. Sánchez-Friera, and R. W. Godby
Self-consistent calculations of the total energies of electron systems using many-body theory

10:15–10:30 Stefan Kurth, John P. Perdew, Aleš Zupan, Peter Blaha
Accurate density functional with correct formal properties: A step beyond the generalized gradient approximation

10:30–11:00 L. Vitos, B. Johansson, J. Kollár, H. L. Skriver
Kinetic and exchange functionals in the local Airy gas approximation

11:00–11:30 Coffee

11:30–12.00 J.G. Snijders, F. Kootstra, P.L. de Boeij
Time dependent density functional theory in extended systems

12:00–12:15 Jiang Wang
Solving the self-consistent Kohn-Sham equations with a nonlinear numerical algorithm

12:15–12:30 Robert K. Nesbet
Orbital-functional theory as an exact N-electron model

Friday Morning Session, Ratgeb room: MOL/BIOL
Chair: F. Seno

09:30–10:00 B. Lesyng
Mesoscopic Poisson-Boltzmann and quantum-classical studies of enzymatic-reaction

10:00–10:15 Joel Ireta, Jörg Neugebauer, Matthias Scheffler, Arturo Rojo, Marcelo Galván
Strain induced phase transition of an alpha-helix: the interplay between hydrogen bonds and peptide planarity

10:15–10:30 H. M. Petrilli, B. Ctortecka, W. Tröger, T. Butz
Electric field gradients in metal complexes with biological applications

10:30–11:00 Coffee

11:00–11:30 Ursula Röthlisberger
First-principles modeling of enzymes

11:30–12:00 Paolo Carloni
Drug-target interactions in anti-AIDS therapy: an ab initio approach

12:00–12:30 M.D. Segall, M.C. Payne, P.J. Eddershaw
An ab initio study of cytochrome P450 enzymes: understanding and predicting drug metabolism

12:30–14:00 Lunch

Friday Afternoon Session, Baldung room: CORR-SYS
Chair: R. Martin

14:00–14:15 E. Koch and Stefan Goedecker
Decay properties of the density matrix and Wannier functions for interacting systems

14:15–14:30 H. Rosner, S.-L. Drechsler, K. Koepernik, R. Hayn, and H. Eschrig
The electronic structure of $CuSiO_3$ - a possible candidate for a new inorganic spin-Peierls compound?

14:30–15:00 O. Gunnarsson and J. Han
Resistivity of alkali-doped fullerenes: Lack of saturation at high temperatures?

15:00–15:30 Abhijit Mookerjee, Tanusri Saha-Dasgupta
An augmented space recursive approach to the solution of the Hubbard model

15:30–16:00 S. Yu. Ezhov, V. I. Anisimov, D. I. Khomskii, G. A. Sawatzky
Orbital occupation, local spin and exchange interactions in V_2O_3

16:00–16:30 Coffee

Friday Afternoon Session, Parler room: SEMIC
Chair: M. Scheffler

14:00–14:30 P. Kratzer and M. Scheffler
From DFT studies to growth simulations: Modeling molecular beam epitaxy of arsenide compound semiconductors

14:30–15:00 M. Pesola, Y. J. Lee, R.M. Nieminen, J. von Boehm
Oxygen-related defects in Si and GaAs

15:00–15:15 P. Wahnón, J. Fernández, and C. Tablero
Electronic structure calculations for new photovoltaic materials

15:15–15:30 C.J. Fall, R. Jones, P. R. Briddon, S. Öberg
Electronic and vibrational properties of Mg- and O-related complexes in GaN

15:30–16:00 Chris G. Van de Walle and J. Neugebauer
Properties of GaN surfaces: the role of hydrogen

16:00–16:30 Coffee

Friday Afternoon Session, Ratgeb: OEP
Chair: E.K.U. Gross

14:00–14:30 Andreas Görling
Advances in DFT by treating exchange exactly

14:30–14:45 Andrzej Fleszar
Exact exchange (EXX) and GW calculations of the electronic structure of semiconductors

14:45–15:00 Y.-H. Kim
Exact-exchange-based hybrid-method investigations of small molecules

15:00–15:30 E. Engel, A. Höck, and R. M. Dreizler
Description of dispersion forces with implicit density functionals

15:30–16:00 Michael Seidl, John P. Perdew, Stefan Kurth
Strong-interaction limit of density functional theory: its simplicity and its relevance for electron systems

16:00–16:30 Coffee

Friday Late Afternoon Session, Baldung room: EXC/QP
Chair: O. Gunnarsson

16:30–17:00 Steven G. Louie
Ab initio optical absorption spectra

17:00–17:15 Arno Schindlmayr
Decay properties of the one-particle Green function in real space and imaginary time

17:15–17:30 Atsushi Yamasaki and Takeo Fujiwara
Quasiparticle properties of transition metals in the GW approximation

17:30–18:00 Walter Wolf, Sandro Massidda, Michele Posternak, Jürgen Sticht, and Erich Wimmer
Screened exchange FLAPW calculations of optical properties

18:00–18:15 M. Fuchs, X. Gonze, T. Klüner, and M. Scheffler
Potential energy surfaces of excited states from time-dependent density-functional theory

18:15–18:30 P. van Gelderen, P.A. Bobbert, P.J. Kelly, and G. Brocks
Parameter-free quasi-particle calculations for YH_3

18:30–19:00 R. Del Sole, G. Onida, P. Monachesi, M. Palummo
Ab-initio calculation of optical properties of surfaces

Friday Late Afternoon Session, Parler room: MATER
Chair: J. Kollar

16:30–16:45 S. I. Simak, U. Häussermann, S. Lidin, R. Ahuja, and B. Johansson
Group-III metals under high pressure: a unified bonding picture

16:45–17:00 R. Hirschl, J. Hafner, Y. Jeanvoine
Ab initio phase diagram of palladium-vanadium alloys

17:00–17:30 Mike Gillan, Dario Alfè, and David Price
How to find the chemical composition of the Earth's core using DFT

17:30–17:45 K. Carling, G. Wahnström, T. R. Mattsson, A. E. Mattsson, N. Sandberg, G. Grimvall
Vacancies in metals: from ab-initio calculations to experimental data

17:45–18:00 M. Alatalo, M. Weinert
Defect–defect interactions in Al

18:00–18:30 Niels E. Christensen
New high-pressure phases of alkli metals and semiconductors

18:30–18:45 Barbara Montanari and Michael W. Finnis
Alumina: a tight-binding model with polarisable ions

18:45–19:00 F. Lechermann and M. Fähnle
Ab-initio statistical mechanics for ordering phenomena and phase diagrams of compounds including the effect of vacancies

Friday Late Afternoon Session, Ratgeb room: MAGNET-EL
Chair: H. Dreyssé

16:30–17:00 A. Barthélémy, J.M.De Teresa, A.Fert, J.P.Contour
F.Pailloux, J.L.Maurice, M.Bowen, A.Vaures
Magnetic tunnel junctions : experimental results and open questions

17:00–17:30 W.H. Butler, X.-G. Zhang, T. C. Schulthess, J. M. MacLaren
Spin dependent tunneling in Fe|MgO|Fe

17:30–18:00 N. Papanikolaou, Ph. Mavropoulos, M. Freyss, R.Zeller,
and P.H. Dederichs
Spin dependent transport in metal-insulator junctions

18:00–18:15 Claudia Blaas, Peter Weinberger, Laszlo Szunyogh, Peter M. Levy,
and Charles Sommers
Theoretical evaluation of magnetotransport properties in Co/Cu/Co-based spin-valves

18:15–18:30 H. Akai, T. Kamatani, and S. Watanabe
Electronic structure and magnetism of diluted magnetic semiconductors

18:30–19:00 E. Y. Tsymbal
Spin polarization of conductance in magnetic tunnel junctions

Friday Evening Session

19:45–20:15 Organ concert, Münster

Saturday, 26 August 2000

Saturday Morning Session, Parler room: Plenary
Chair: P.H. Dederichs

08:30–09:25 Peter M. Levy
Magnetotransport in multilayered structures

Saturday Morning Session, Baldung room: MOL/BIOL & POLYM
Chair: C. Koenig

09:30–10:00 Carme Rovira and Michele Parrinello
Ligand binding properties of myoglobin modeled by first principles molecular dynamics

10:00–10:30 Emilio Artacho
Large scale calculations on DNA and proteins

10:30–11:00 Coffee

11:00–11:30 A. Ruini, F. Rossi, E. Molinari, R.B. Capaz, and M.J. Caldas
Ab-initio study of Coulomb-correlated optical properties in conjugated polymers

11:30–12:00 Bernard Delley
Structural switching in condensed molecular complexes triggered by optical excitations

12:00–12:15 Flavio Seno
Learning effective energy functions for protein structure prediction

12:15–12:30 Michael Springborg
Modifying polyacetylene

Saturday Morning Session, Parler room: MAGNET-EL
Chair: P.H. Dederichs

09:30–10:00 I. Mertig, J. Binder, and P. Zahn
The phenomenon of giant magnetoresistance: an ab initio description

10:00–10:30 Coffee

10:30–11:00 J. Kudrnovský, V. Drchal, I. Turek, C. Blaas, P. Weinberger, and P. Bruno
Ab initio theory of perpendicular transport in layered magnetic systems

11:00–11:15 I. Riedel, P. Zahn, and I. Mertig
Transmission coefficients - a new formalism

11:15–11:30 Peter Zahn and Ingrid Mertig
Ab initio description of TMR electrodes Fe, Co, and Ni

11:30–11:45 I.I. Oleinik, E.Yu. Tsymbal, and D.G. Pettifor
Structural and electronic properties of $Co/Al_2O_3/Co$ magnetic tunnel junction from first-principles

11:45–12:00 K. Xia, P. J. Kelly, G. E. W. Bauer, I. Turek, J. Kudrnovský, and V. Drchal
Interface resistance of disordered magnetic multilayers

12:00–12:30 I.I. Mazin
Is spin polarization a measurable quantity?

Saturday Morning Session, Ratgeb room: SUPERC
Chair: O.K. Andersen

09:30–10:00 Z. Szotek, B. L. Gyorffy, W. M. Temmerman, O. K. Andersen, and O. Jepsen
Quasiparticles in d-wave superconductors

10:00–10:30 James F. Annett
Exotic superconductors

10:30–10:45 M. Lüders, M. Marques, L. Fast, E. K. U. Gross
Strong electron-phonon coupling in the density functional theory for superconductors

10:45–11:00 E.G. Maksimov and D.Yu. Savrasov
Dynamical stability, electron-phonon interaction and superconductivity in hydrogen at high pressure

11:00–11:30 Coffee

11:30–12:00 David J. Singh and Igor I. Mazin
Is singlet and triplet superconductivity incompatible?

12:00–12:30 Klaus Capelle
Relativistic effects and dichroism in superconductors

12:30–14:00 Lunch

Saturday Afternoon Session, Baldung room: F-EL
Chair: L. Sandratskii

14:00–14:45 A. Svane, L. Petit, W. Temmerman, Z. Szotek, P. Strange, and H. Winter
Self-interaction corrected electronic structure of lanthanides and actinides

14:45–15:00 L. Petit, A. Svane, W.Temmerman, Z. Szotek
Electronic structure of americium compounds in the self-interaction corrected local-spin-density approximation

15:00–15:15 M. Pénicaud
Calculated equilibrium properties, electronic structures and structural stabilities of Th, Pa, U, Np and Pu

15:15–15:30 C. J. Pickard, B. Winkler, R. K. Chen, M. H. Lee, J. S. Lin, M. C. Payne, J. A. White, V. Milman, and D. Vanderbilt
Structural properties of lanthanide and actinide compounds within the planewave pseudopotential approach

15:30–16:00 Coffee

Saturday Afternoon Session, Parler room: EXC/QP
Chair: R. Del Sole

14:00–14:30 Lucia Reining and Valerio Olevano
Application of Green functions methods to the calculation of excited states

14:30–14:45 Michael Rohlfing and Johannes Pollmann
Surface excitons at the Si(111)-(2x1) surface

14:45–15:00 M. Kuzmin, C.D. Hogan, and C.H. Patterson
Quasi-particle band structures of wide-gap insulators

15:00–15:30 A. Rubio, I. Campillo, J. M. Pitarke, V. M. Silkin, E. V. Chulkov, P. M. Echenique
Lifetime of hot electrons in metals

15:30–16:00 Coffee

Saturday Afternoon Session, Ratgeb: SUPERC
Chair: E. Maksimov

14:00–14:30 Eva Pavarini, O. Jepsen, and O. K. Andersen
Hyperfine fields in cuprate superconductors

14:30–14:45 Claudia Ambrosch-Draxl, Pavel Korzahvyi, and Börje Johansson
Ab initio study of the oxygen orderig in $YBa_2Cu_3O_{7-x}$

14:45–15:00 C. Franchini, S. Massidda, A. Continenza, A. Gauzzi
Structural and electronic properties of $Hg_{1-y}Mo_yBa_2CuO_{4+\delta}$

15:00–15:15 Barry M. Klein
Instabilities in A15 compounds: A first-principles study

15:15–15:30 P. Süle and C. Ambrosch-Draxl
Hole doping in the $HgBa_2CuO_{4+\delta}$ *high* T_c *superconductor*

15:30–16:00 Coffee

Saturday Late Afternoon Session, Baldung room: F-EL & MAGNET
Chair: H. Eschrig

16:00–16:30 M.S.S. Brooks
Relativistic effects in f-electron systems

16:30–16:45 P. M. Oppeneer, T. Kraft, M. S. S. Brooks
Electronic structure of plutonium monochalcogenides

16:45–17:00 L. M. Sandratskii
Incommensurate magnetic structures in relativistic systems

17:00–17:30 Lars Nordström
Magnetism of the rare earth from first principles calculations

17:30–17:45 L. Steinbeck, M. Richter, and H. Eschrig
Itinerant-electron magnetocrystalline anisotropy energy of rare-earth transition-metal intermetallics from density functional calculations

17:45–18:00 Stefaan Cottenier and Heinz Haas
Hyperfine fields and local relaxations for impurities in bcc Fe: an FLAPW study

Saturday Late Afternoon Session, Parler room: QMC
Chair: E. Koch

16:00–16:30 R.J. Needs, A.R. Porter, M.D. Towler, Y. Lee, W.K. Leung, G. Rajagopal, P.R.C. Kent, R.Q. Hood, W.M.C. Foulkes, S. Itoh, and S. Ihara
Accurate QMC calculations for ground and excited states

16:30–17:00 Claudia Filippi
Energy derivatives in quantum Monte Carlo: forces and optimization

17:00–17:30 Michel Caffarel
Zero-Variance principle for classical and quantum Monte Carlo algorithms

17:30–18:00 F. Becca, L. Capriotti, and S. Sorella
Stability of d-wave superconductivity in the t-J model

Saturday Late Afternoon Session, Ratgeb room: MATER
Chair: B. Winkler

16:00–16:15 A. V. Postnikov, P. Entel, P. Ordejón
Structure and electronic properties of non-metallic surfaces and nanoparticles

16:15–16:30 M. Šob, L.G. Wang, V. Vitek
Theoretical tensile strength in metals and intermetallics

16:30–17:00

17:00–17:15 H.G. Salunke, G.P. Das, S.N. Mishra, A.A. Tulapurkar, R.G. Pillay, and S. Cottenier
Electronic structure and magnetic properties of Mo impurities n Yb-host

17:15–17:30 R.I. Eglitis, E.A. Kotomin, and G. Borstel
Computer modelling of ABO_3 perovskites

17:30–17:45 W. Münch, K.-D. Kreuer, J. Maier, G. Seifert
Investigation of the proton diffusion mechanism in liquid imidazole using ab initio and quantum molecular dynamics simulations

17:45–18:00 K. Parlinski
Ab initio calculations of lattice dynamics and phase transitions

Saturday Early Evening Session, Parler room: SUMMARY
Chair: O.K. Andersen

18:05–18:35 V. Heine
Summary of the Conference
18:35–18:45 P.J. Durham
Closing of the Conference

Psi-k2000 Conference: Concluding Remarks

Volker HEINE
Cavendish Laboratory, Madingley Road, Cambridge CB3 0HE, England

It has been a fantastically good conference. A conference is made by the participants, even more than by the speakers and organisers, and on the first two nights after the poster sessions I estimate that a quarter of the people were still around discussing when the building custodian was wanting to lock up at 11pm. Already before arriving here, in fact last November, you had made a big contribution by sending in over 500 suggestions for invited speakers, and this has resulted in a very very high quality programme. I was constantly dashing between the three parallel sessions, and although I think staggering the coffee breaks is an excellent idea, it meant that I often did not get my coffee because I did not want to miss one of the talks!

So continuing the theme that it is the participants that make the conference, let me start with the posters and contributed talks. The first impression is of the enormous range of topics covered, many old ones ['old' in our subject means perhaps five years old!] and many new ones. An example is having a whole symposium on applications to biology, a subject that I don't think existed at all in our 1996 conference. One could cite the polymer symposium too, and an explosion in the number of papers on oxides. The magnetism work has also developed enormously, with non-collinear polarisation of the atoms, and with complex nano-structures of multi-layers.

So my first comment is that there is no doubt that our methodology is opening doors to many new avenues of research that would not be possible without it. Again and again I heard a speaker say that some data did not make any sense to the experimentalists and they asked for the calculations to clarify the situation [which they did];, or that there were three different possible interpretations of the data and only our calculations could decide which was the correct one.

My second observation is the striking degree of realism now in the simulations. The title of Philip Lindan's Euresco conference next year says it all: "From out of the vacuum into the real world". This was in evidence almost everywhere in the close interaction with experiment.

Thirdly I noted a whole new emphasis on not just calculating structures and energies, but in simulations of many different probes that experimentalists use and that need calculations to

interpret them. In some cases the calculations allow a bit of extra certainty or information to be extracted from the observations, but in other extreme cases the data are totally useless without a substantial parallel computer simulation.

Fourthly I saw evidence everywhere of the technical improvements and speed-up of the calculations, without which much of the work could not have been done.

Many of the contributed papers and posters are what I would call 'bread and butter' calculations, calculations of a type now fairly common but applied to some valid scientific project [and carried out at a very high standard of quality]. That is alright. Almost all science is 'bread and butter' science. These days there is an enormous status attached to 'novelty', which I think is sometimes artificial and often misplaced. In the 1960s Kuhn wrote an important book on how science actually progresses, pointing out how there were occasional 'breakthroughs' [which he called 'revolutions'] which then led to whole new fields of what he described as 'normal science'. It is not much use having a breakthrough if no-one then follows through with exploiting it to achieve new scientific understanding.

For me the breakthrough came in 1978 when Richard Martin and Marvin Cohen with their groups showed that with pseudopotentials and plane waves one could do simulations calculating Hellmann-Feynman forces and getting reliable energy differences between structures. Around the same time there were similar great advances in magnetism, in the KKR and LMTO formalisms, and with Augmented Plane Waves. All that we have today has sprouted from those beginnings, with an enormous boost provided by Car and Parrinello. So from our perspective we already have a maturity of 20 years since that time. But as far as our impact on the rest of science is concerned, I think we have only seen the beginnings.

Let me give a few examples and make a few comments about our impact on the rest of science.

One of the places where one can see that impact is in the pages of Physical Review Letters, of course the highest prestige journal in physics in all the world. Last April I had occasion to look through the then latest issue of Phys. Rev. Lett., which I think was fairly typical, and I counted 5 papers out of the total of 52 from the whole of physics [not just condensed matter] based on what is becoming known as our psi-k methodology. In other words we are 10 percent of all physics at the forefront of research that gets into PRL, not 10 percent of all physics generally but 10 percent of the leading edge. Of these five papers, two came from Europe, two from USA and one from Japan. The engagement with main-stream science and even technology is shown by the opening words of one of those papers [from Scheffler's group]: "The nature of the corundum surface (alpha aluminium oxide) is of considerable importance in a wide variety of technological applications. These range from catalytic supports and thin-film substrates to corrosion and wear protection in mechanical systems." Incidentally I am grateful to Scheffler for that bit of propaganda. We need to 'sell' ourselves a bit: remember how the high energy particle physicists are always boosting their funding by claiming to "discover the secrets of the universe".

Another great piece of propaganda which we can all take pride in is the work of Gillan's group appearing on the main evening television news in Britain. That was the calculation of properties and chemical partitioning at the earth's core which he spoke about here.

I also can point to the fact that our community stimulates one Euresco conference per year, when other areas have an interval of at least two years and there are only about five or six in the whole of physics in a year. How does it come that we are so prominent? The answer is that we are the vanguard! Our conferences move around different fields such as surface science or magnetism or semiconductors etc, and they involve the experimental side and theory as well as our computations, but it is our computational methodology that is opening new doors which puts it at the centre of these conferences.

Another trend that I notice in this regard is how people from our community are moving into jobs in all sorts of research institutes. Recently I came across one in a laboratory for research on glasses, and another in a geological institute. Both of them are in an important country where however the leaders in theoretical physics have a strong prejudice against computational physics so that there is no leading group in that country in our type of work. The point is that the experimentalists are saying they need us, no matter what the professional theoreticians may think.

Another evidence of the realism of our calculations comes from the fact that there are 9 invited talks from industry and at least one contributed talk, with several more containing an industrial co-author. For example, just to pick one, there was Dr Toulhoat's talk on the catalyst for desulphurisation of petroleum and how it works. The interaction of basic research and industry is very complicated, with very different patterns in different situations. Let me just make a few brief remarks. There is no doubt that our methodology will find increasing application in industry, but it is well to remember the time lag of typically 10 to 40 years in physics between basic research and industrial application, though this can be much shorter in chemistry and the bio-medical world. For example ab initio simulations have already been used in the search for biomimetics, which are simpler molecules that mimic the behaviour of some complicated macromolecular agent. One can often see quite a long chain starting with basic science which feeds into applied research which leads to development and then ultimately perhaps to industrial use or production. Our work is often near the beginning of such a chain, but is none the less valuable for that. If there is nothing going into the beginning of the chain, there will not be anything coming out the end, which is a point worth stressing when we are under pressure to be 'relevant'. One of the ways that basic science is often used in industry is in trouble shooting, which applies over the whole range from low-tech to high-tech industry. My father was technical manager of a pottery factory making vases and dinner sets etc.. I remember one day it happened that the cups came out of the tunnel kiln with their handles dropped off: what to do? Even stopping putting new ware into the kiln would disturb its temperature regulation, and I could see that all the ceramic science that my father knew became relevant in analysing the possible causes, interpreting symptoms, doing some quick tests and finally correcting the problem. Much of the science that he used was from research 40 years earlier, but some was quite recent. We can also see the aspect of trouble shooting in the talk by P.Bloechl from IBM at Zuerich, where he spoke about stress-induced leakage current in semiconductor devices due to hydrogen impurity.

I now turn to the invited talks and new advances. One notable feature is how many-body theory is making contact with real materials and our type of calculations, and not just dealing with very simplified model systems. For example I saw three times at this conference the comparison between the measured and calculated band gaps of semiconductors from three different approaches

to calculating the many-body corrections. All the results were very good, incidentally.

Another new development is the calculation of electron transport which is now standard, for example in the magnetic multi-layer devices. At our previous conference in 1996 that had hardly started.

I have already mentioned the applications to biological systems, which I think did not exist at Psi-k1996 but has a full symposium at the present conference.

Extending the length and time scales of our simulations is of great importance. I was told about one of the pseudopotential/plane-wave codes that it is now about 10 times faster than five years ago due to algorithmic improvements. As regards the length scale, we have seen the spectacular increase to 16 000 silicon atoms reported by Bowler and Gillan, and also an impressive expansion by the Siesta code. That is still a very active area of research, and it is still far from certain what finally the approach will be. I know there has been an enormous interest in the 'order N problem' but I think that lengthening the time scale would have even more important consequences for our work.

Finally the work of Resta and Vanderbilt has added a whole new dimension to our way of thinking about basis states and their localisation. It turns out that localisation is not just some arbitrary choice of representation, but that deep in the physics there is information about the right and wrong way of thinking about localised electrons in a specific material.

Finally I want to say a little bit about the infrastructure that supports our community in Europe and has made this conference possible for example. People get a bit confused because it is confusing. There is no permanent or renewable source of funding, and so we go from one type of programme to another at one agency or another, adapting ourselves to whatever the funding agencies want. Supporting this conference and this Psi-k Newsletter are two Brussels EU TMR Networks which also alone or jointly with the ESF Programme (see below) run some workshops, but they can only pay for travel etc for people directly connected with the nodes written into the contract which we drew as wide as we could without sinking them.

Of much wider scope is the European Science Foundation (ESF) Psi-k Programme which is subscribed to by 17 nations, and anyone working in any of those nations is ***automatically*** entitled to participate in the sense that the s(he) can apply for financial support: there is no further 'membership' of the programme. The list of countries can be found on our web page

http://psi-k.dl.ac.uk/

and includes all western Europe except Greece, The Netherlands, and Norway. People from other countries including Russia and Ukraine can also apply if they have an invitation from an institution which is in one of the 17 countries.

The activities run by the ESF Psi-k Programme, apart from this conference, includes workshops, tutorial sessions with hands-on training in one or another code, this Psi-k Newsletter, and individual bilateral visits. All are explained on the web site given above. The individual visits may be for any valid research purpose, such as starting or continuing a collaboration, or learning a piece of expertise, or training in the use of a code. The purpose of the visitor scheme is especially to help young researchers and those in more isolated research groups. Obviously we cannot pay for all the travel of all the people represented here at this conference, and so a necessary condition

is that other funding is not available. In such cases the method of application is very quick and non-burocratic: see the web page [which has recently been upgraded so that it is not always easy to find the relevant information, but this is expected to be straightened out soon]. Note that there must be a report of the visit submitted to the Newsletter before you can claim your money.

Now we come to an IMPORTANT MESSAGE. We will soon start the process of applying for new ESF funding from January 2003, ie from the end of the present Programme. The bad news is that at the right time we will notify everyone and you will have to apply pressure on your own national research council to approve the proposal and to join it, ie to put money into it. Such money comes out of the normal research budget for funding national research, so that national organisations are not keen to join unless persuaded that it is important for researchers in their countries. However the good news is that it is all not very expensive when divided between 17 countries. So I hope that you/we will be successful, because I really do believe that the various schemes for collaboration that there have been over the last 20 years have helped to make our type of research flourishing in both quality and extent in Europe.

I will now hand over to Paul Durham, the conference chairman, and no doubt he will mention to you the people who have done the many tasks necessary to the smooth running of this conference. I think the arrangements have been excellent. But I would like to just add my personal deep thanks to Paul for stepping in four years ago at the end of our first conference and offering to take on the responsibility, when there was no funding in place, of making sure that somehow this conference would happen. And I also want to pay tribute to Walter Temmerman and Dzidka Szotek who have worked tirelessly for many months for the conference. Please join me in expressing our heartfelt thanks.

3 News from the TMR1 Network

"Interface Magnetism"

3.1 Workshop Announcements

3.1.1 Workshop on GMR and TMR

TMR-Network Magnetoelectronics

Dresden

November 30th - December 03rd, 2000

Purpose: Presentation and discussion of results and concepts to elucidate the microscopic origin of GMR, TMR and related phenomena

Arrival: Thursday, November 30th, 2000

Departure: Sunday, December 03rd, 2000

We plan to have longer contributions (40 minutes) and short contributions (20 minutes) + discussions starting Friday morning, Saturday and Sunday morning.

Requirements:

Please confirm your participation by sending me an e-mail indicating the accompanying guests and any request concerning the accomodation until

October 10, 2000.

Please fill out the following form and e-mail it back to:

mertig@theory.phy.tu-dresden.de

Name:
Postal Address:
Telefon/Fax:
e-mail:
Share room with:
Title of your contribution, if any:

Please send me a short abstract in latex form for each contribution, suitable to be presented in the Ψ_k-Newsletter, until

October 10, 2000.

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3.1.2 XRMS-2000 Workshop

International Workshop on X-ray Spectroscopies for Magnetic Solids 2000 (XRMS-2000)

On December 9th, 2000, in only 50 working days from now we will come together for the

International Workshop on X-ray Spectroscopies for Magnetic Solids (XRMS-2000),

held at Berlin, Germany.

For those who have not registered until now we like to remind you that the REGISTRATION DEADLINE is Friday, October 6th. You may either register by Fax, using the appended form (regiform.ps), or by email. Please supply your name, institution, and nationality (in capital letters), as it shall appear on your name tag during the workshop.

If you intend to present a poster, please include the title and a half page ABSTRACT, which we will distribute among the XRMS-2000 participants.

We should also like to remind all SPEAKERS to send their abstract by October 6th.

Attending the workshop banquet at Saturday night will be free of charge for all participants who have registered by 6th October. For latecomers and for accompanying persons there will be a banquet fee of DM 40.

For those who come from abroad, it may be of interest to note that in the week Dec. 11-14, right after XRMS-2000, there will by the DPG-Symposium on occasion of the 100th anniversary of Quantum mechanics at Berlin, Germany. For details, please see

http://www.dpg-physik.de/kalender/qt100/symp/symp.htm?/kalender/qt100/symp/sy2co.htm

Please do not hesitate to contact either Kai Starke or Hubert Ebert for further information. The XRMS-2000 website is:

http://www.physik.fu-berlin.de/ starke/xrms2000/

SCOPE:

The international workshop on x-ray spectroscopies for magnetic solids shall bring together theoretical and experimental scientists who involve themselves in the developments of x-ray spectroscopies for magnetism research. The one-day meeting provides an opportunity to discuss current advances in the field, as well as to visit the German synchrotron-radiation facility BESSY 2 at Berlin.

DATE:

Saturday, 9 December 2000, after BESSY-user meeting.
Begin: 9:00; end: 19:00. Afterwards: Workshop dinner.

VENUE:

Berlin, Germany, Synchrotron-Radiation Facility BESSY 2, Berlin-Adlershof (see http://www.bessy.de)

SCIENTIFIC PROGRAMME:

Several invited lectures as well as contributed talks and posters.

INVITED SPEAKERS:

G. van der Laan (Daresbury)
L. Braicovich (Milano)
J. B. Kortright (LBNL)
J. Tobin (LLNL)
E. Dudzik (HMI)
H. Wende (FU Berlin)
T. Eimueller (Wuerzburg)
J. P. Hill / C.-C. Kao (BNL) (*)
M. Blume (BNL) (*)
C. Vettier (ESRF) (*)
C. Natoli (Frascati) (*)
P. Strange (Keele)
Y. U. Idzerda (NRL) (*)
W. Kuch (Halle) (*)
J. Minar (LMU Muenchen)
F. Heigl (FU Berlin)

(*) : to be confirmed

ORGANIZERS:

PD Dr. K. Starke (Berlin) Prof. Dr. H. Ebert (Muenchen)

REGISTRATION/FEES:

Registration shall be made by October, 6th, 2000. Electronic registration is preferred (via email to: starke@physik.fu-berlin.de or he@gaia.cup.uni.muenchen.de). No fees. Unfortunately we cannot support your travel.

ABSTRACT:

An up to half-page abstract shall be submitted for every invited and contributed presentation (posters included). It will be distributed amoung all participants of XRMS-2000 two weeks before the workshop.

FURTHER INFORMATION:

Please see:

http://www.physik.fu-berlin.de/ starke/xrms2000/

This site will be update regularly.

SUPPORTED BY EUROPEAN TMR-NETWORK:

Ab-initio Calculations of Magnetic Properties of Surfaces, Interfaces and Multilayers.

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4 News from the Research Training Network (RTN)

COMPUTATIONAL MAGNETOELECTRONICS

4.1 Young Researcher Positions

Daresbury - Bristol - Juelich - Muenchen - Halle - Paris - Vienna - Twente - Uppsala - Brno - Budapest - New York

We have positions for several Young Researchers to work on an EU funded Network to model, understand and predict the electronic, magnetic and transport properties of materials and material systems relevant to magnetoelectronics. These positions are available from 1st October 2000.

The scientific projects are:

- **Ferromagnet/ Semiconductor Interface**. For more detail please contact Susanne Mirbt (susanne@fysik.uu.se)
- **Ferromagnet/ Oxide Interface**. For more detail please contact Patrick Bruno (bruno@mpi-halle.de)
- **Ferromagnet/ Superconductor Interface**. For more detail please contact Balazs Gyorffy (b.gyorffy@bristol.ac.uk)
- **Magnetic Nanostructures**. For more detail please contact Laszlo Szunyogh (szunyogh@dirac.phy.bme.hu)
- **Magnetooptics**. For more detail please contact Mebarek Alouani (mea@Taranis.u-strasbg.fr)
- **Magnetic X-ray Scattering**. For more detail please contact Walter Temmerman (w.m.temmerman@dl.a
- **Giant Magnetoresistance**. For more detail please contact Peter Weinberger (pw@cms.tuwien.ac.at)
- **Tunneling Magnetoresistance**. For more detail please contact Peter Dederichs (l.gerken@fz-juelich.de)
- **Spin Mesoscopics**. For more detail please contact Paul Kelly (p.j.kelly@tn.utwente.nl)
- **Experiment**. For more detail please contact Albert Fert (fert@lps.u-psud.fr)

A copy of the proposal including the scientific projects can be found on

http://psi-k.dl.ac.uk/Magnetoelectronics/default.html .

The Network activily encourages the application of female researchers. Nine senior researchers in the Network are female.

If you wish to find out more detail please contact Walter Temmerman (w.m.temmerman@dl.ac.uk) or Peter Dederichs (l.gerken@fz-juelich.de).

The EC Rules for Young Researchers are that the Researcher must be:

1. aged 35 years or less at the time of appointment by a participant. An allowance to this age limit may be made for the actual time spent in compulsory military or civil service or child care (a maximum of two years per child for the actual time spent off work);
2. a holder of a doctoral degree or enrol on a Ph.D. course;
3. a national of a Member State of the Community or of an Associated State or have resided in the Community for at least five years prior to appointment by a participant in the frame of this contract;

and must not be:

1. a national of the state in which the participant's research appointing team is located and must not have carried out their normal activities in that state for more than 12 of the 24 months prior to appointment.

Details of the those countries which are defined as "Associated States" (such as Bulgaria, Czech Republic, Estonia, Hungary, Latvia, Lithuania, Poland, Romania, Slovakia, Slovenia) may be found at:

http://www.cordis.lu/fp5/src/3rdcountries.htm

4.2 Workshop Announcements

4.2.1 EGSCM PRAGUE'01

European Graduate School on Condensed Matter (EGSCM)
"Physics of Magnetic Multilayers - Theory and Experiment"

Below you will find information concerning the European Graduate School on Condensed Matter (EGSCM) to be organized in Prague in June 2001. We will appreciate if you would inform potential applicants (PhD students and young postdocs) interested in the subject of metallic multilayers. All necessary information on the EGSCM is available and will be continuously updated at the web-site:

http://195.113.32.128/EGSCM_Prague.htm

TITLE AND PURPOSE

The European Graduate School on Condensed Matter (EGSCM Prague'01) will follow the initiative of colleagues at IFW Dresden (February 2000). The EGSCM Prague'01 offers a course on: Physics of Magnetic Multilayers - Theory and Experiment. The course is aimed at introducing graduate and PhD students of condensed matter physics and materials science to the state-of-the-art of important topics of current research. Subjects of scheduled lectures fall into three main categories:

(i) Electronic structure of multilayers and its experimental study
(ii) Exchange interactions and relativistic effects in multilayers
(iii) Spin-dependent transport in multilayers

The EGSCM will be organized by the Charles University in Prague (Department of Electronic Structures), the Academy of Sciences of the Czech Republic (the Institute of Physics, Prague and the Institute of Physics of Materials, Brno), and the Czech node of the RTN Network on Computational Magnetoelectronics.

Main organizer:

Prof. V. Sechovský (sech@mag.mff.cuni.cz)
Department of Electronic Structures
Faculty of Mathematics and Physics

Charles University
Ke Karlovu 5
121 16 Praha 2, The Czech Republic

Programme commitee:

Dr. V. Drchal (drchal@fzu.cz) and Dr. J. Kudrnovský (kudrnov@fzu.cz)
Institute of Physics
Academy of Sciences of the Czech Republic
Na Slovance 2
182 21 Praha 8, The Czech Republic

and

Dr. I. Turek (turek@ipm.cz)
(Leader of the Czech node of the RTN Network on Computational Magnetoelectronics)
Institute of Physics of Materials
Academy of Sciences of the Czech Republic
Žižkova 22
616 62 Brno, The Czech Republic

SCIENTIFIC CONTENT

Magnetic multilayers are artificially prepared materials with unique physical properties and of great application potential and interest (magnetoelectronics). Conventional workshops and conferences devoted to this "hot" subject are now regularly organized (e.g., the conference on multilayers to be held in Aachen in 2001). We feel a need for a similarly oriented school with tutorial accounts of current problems on a high scientific level engaging leading persons in the field.

LIST OF LECTURERS AND SUBJECTS OF LECTURES

Following speakers listed below agreed to participate at the EGSCM and to deliver an invited lecture on a subject of their expertise.

(i) **General properties and electronic structure**

1. B. Velický (Charles University): *Introduction into the electronic structure*
2. H. Eschrig (IFW Dresden): *Introduction to the Density Functional Theory*
3. B.L. Gyorffy (University of Bristol): *Magnetism of metals*
4. P. Dederichs (FZ Jülich): *Electronic structure of magnetic metal surfaces*

5. I. Turek (Academy of Sciences, Brno): *Electronic structure of random magnetic metals and their surfaces*
6. J. Henk (Halle): *LEED and photoemission from ultrathin magnetic films*
7. J. Hafner (University of Vienna): *Non-collinear magnetism*
8. A. Lichtenstein (University of Nijmegen): *Magnetism and electronic correlations*

(ii) **Exchange interactions and relativistic effects in magnetic metals**

1. P. Bruno (MPI Halle): *Theory of exchange interactions in metals and multilayers*
2. S. Blügel (FZ Jülich): *Theory of magnetic anisotropy in metals and multilayers*
3. H. Ebert (University of Munich): *Magnetooptical effects*
4. G. van der Laan (Daresbury): *Magnetic circular dichroism: theory*

(iii) **Transport in magnetic multilayers**

1. P.M. Levy (New York University): *Theory of magnetotransport*
2. I. Mertig (TU Dresden): *Ab-initio theory of GMR: Boltzmann equation approach*
3. P. Weinberger (TU Vienna): *Ab-initio theory of GMR: Kubo-Greenwood approach*
4. P. Kelly (University of Twente): *Ab-initio theory of GMR: Landauer-approach*
5. W. Hofer (City University of London): *Ab-initio theory of STM*
6. J. Mathon (City University of London): *Theory of tunneling in magnetic multilayers*
7. C. Lambert (University of Lancaster): *Ferromagnet-superconductor interfaces: transport properties*

(iv) **Experiment on magnetic multilayers**

1. J. Kirschner (MPI Halle): *Preparation and properties of magnetic multilayers and nanostructures*
2. D. Rafaja (Charles University): *Structure of multilayers using X-rays*
3. X.F. Jin (Fudan University, Shanghai): *Magnetism of 3d-metals and alloys on semiconductors: experiment*

4. C. Carbone (FZ Jülich): *Photoemission from magnetic films*

5. P. Grünberg (FZ Jülich): *Interlayer exchange coupling in metals: experiment*

6. R. Allenspach (IBM Zürich): *Surface Magnetic Anisotropy: experiment*

7. G. Schütz (Würzburg): *X-ray magnetic dichroism: experiment*

8. P. Varga (TU Vienna): *STM from metallic magnetic surfaces: experiment*

9. B. Heinrich (Simon Fraser University): *CIP-GMR and spin relaxation processes: experiment*

10. A. Fert (Thomson): *CPP-GMR and tunneling in multilayers: experiment*

VENUE

Prague, the seat of the oldest university in Central Europe (the Charles University, founded 1348), is one of the most beautiful European towns, the whole city center being declared the UNESCO World cultural monument.

The course will be held in premises of the Center for Graduate and Management Studies (Hotel Krystal, Prague 6) where the Charles University can organize conferences, workshops, schools, etc. at affordable prices of accommodation and hire of lecture rooms. Participants will be accommodated in double rooms at discount prices.

SCHEDULE AND OTHER DETAILS

The EGSCM is planned for 8 days (6 days of school, 1 1/2 days free) from **June 9 through June 16, 2001**. We assume 6 hours of lectures each day. There will be no parallel lectures.

Participants and invited lecturers will be accommodated in the same hotel to facilitate their informal discussions also outside the time of lectures. Poster sessions are planned to enable the participants to present results (also preliminary) of their current research.

PhD students and young post-docs are invited to participate at the EGSCM. A short CV and recommendation of the participant's supervisor will be requested with application. Participants from any country are invited (number of participant is envisaged to be about 40 - 60).

EXPECTED BENEFITS

The school will top experts in this field of research with PhD students and young post-docs from various countries from which, we believe, will benefit participants from both groups. Students and post-docs can get up-to-date knowledge in the field of the course and will develop contacts to experts from leading laboratories and research institutions. Lecturers can benefit from informal discussions with students, who frequently rise new unexpected questions which sometimes may

bring refreshing ideas for future research.

PRELIMINARY APPLICATIONS

We ask interested persons to fill in a simple form given below and to send it via e-mail to **Prof. V. Sechovský** (e-mail: sech@mag.mff.cuni.cz) as soon as possible but not later then by **December 1, 2000**.

PRELIMINARY APPLICATION FORM:

FULL NAME:
UNIVERSITY/INSTITUTE:
ADDRESS:
E-MAIL ADDRESS:
SUBJECT OF STUDY:
SUPERVISOR:
EXPERIMENTALIST: YES/NO
THEORETICIAN: YES/NO
I PLAN TO PRESENT POSTER WITH RESULTS OF MY CURRENT RESEARCH: YES/NO

5 News from the TMR2 Network

'Electronic Structure calculations of materials properties and processes for industry and basic science'

5.1 Mid-term Review Report

TMR Network Title	:	Electronic structure calculations of materials properties and processes for industry and basic sciences
Network Short Title	:	Psi-k
Contract No.	:	ERBFMRXCT98-0178
Commencement date of contract	:	01-03-98
Duration of Contract	:	48 months
Period covered by this report	:	28 months; 01-03-98 - 30-06-00

Name of co-ordinator	:	Dr. Axel Svane
Organisation	:	University of Aarhus
Address	:	Institute of Physics and Astronomy, Ny Munkegade, DK-8000 Aarhus C, Denmark
Telephone	:	+45 8942 3678
Telefax	:	+45 8612 0740
E-mail	:	svane@ifa.au.dk

Network home page : http://www.ifa.au.dk/~svane/tmr-psik.htm

Location of the mid-term review meeting : Schwäbisch Gmünd, Germany

Date and time of meeting : 27-08-00, at 14:30

PART A - RESEARCH RESULTS

A.1 Scientific Highlights

First-principles calculation of the properties of the Nb/α-alumina interface.

The equilibrium structure of the $Al_2O_3(0001)$ surface and the Nb(111)/α-$Al_2O_3(0001)$ interface has been calculated, both in vacuum and with varying partial oxygen pressure, P_{O_2}. The largely ionic nature of the interface bonding has been analysed in terms of bond orders and Mulliken populations. A formalism has been developed, useful for first-principles calculations, which relates the free energy of an oxide/metal interface to the free energies of surfaces and the work of separation of the interface. From total energy calculations for the Nb(111)/α-$Al_2O_3(0001)$ interface, and for free Nb and $Al_2O_3(0001)$ surfaces, the work of separation is numerically determined, which is independent on P_{O_2}. In the next step surface energies, interfacial energies and the equilibrium work of adhesion as a function of P_{O_2} are determined. In the case of Nb/alumina the Al-terminated interface has been identified as the thermodynamically more stable, although mechanically weaker, over most of the range of oxygen pressures considered. However, near the upper range of oxygen pressure (at which the oxide NbO begins to form) the energy difference is too small to be resolved by our present methods.

Simple rules for determining the valencies of f-electron systems.

The self-interaction corrected (SIC) local-spin-density (LSD) computer code has been extended to treat all relativistic effects including spin-orbit coupling. Applications of the scheme to all elemental $4f$ and $5f$ metals and to a large number of f-electron compounds have revealed a simple picture of the effective valency in f-electron systems. The SIC-LSD scheme allows for a splitting of the f electron manifold into localised and band electrons. The number of localised f-electrons is integral, while the number of occupied band f-electrons, n_f, varies continuously, and when this number exceeds a critical value of ~ 0.6, it becomes energetically more favorable to localise an additional f-electron, i. e., the valency of the atom changes by one. The formalism describes correctly the valency changes observed in the series of the $4f$ metals, where Eu and Yb are divalent, while the remaining elements are trivalent, and in the $5f$ metals, where the divalent to trivalent transition takes place between Fm and Es. Similarly, the trends of valency

stability of the $4f$ sulphides are reproduced and follow the same universal picture as the $4f$ elements. An extensive study of Yb compounds, comprising Yb pnictides, chalcogenides and intermetallics, shows that the SIC-LSD formalism is able to describe the entire range of effective valencies from the extreme trivalent, like YbN, to the extreme divalent Yb chalcogenides. A quantitative description of valency changes as a function of pressure is likewise obtained for a series of rare earth compounds, and this has also lead to the identification of some yet unobserved high-pressure phase transitions.

Improved description of excited states

The ab-initio description of excited states in insulating materials is of the utmost importance for the quantitative understanding of the properties of many electronic devices. Results for excitation energies and ionization potentials based upon standard schemes such as LDA or GGA are not sufficiently accurate, for which reason the screened-exchange LDA functional (SX-LDA) has been implemented in a planewave pseudopotential code with parallel and ultrasoft pseudopotential capabilities. The SX-LDA is formulated with a well defined total energy in a perturbative fashion, and full use is made of that capacity to perform molecular dynamics calculations. Fully self-consistent calculations are performed, yielding meaningful ionic forces. In fact, the SX-LDA reduces the self-interaction implicit in LDA which has a major effect in the ionic forces. In particular, the vacancy defects in pure Germanium have been studied. Ge is predicted to be a metal by conventional LDA calculations, which makes it difficult to assess the deep levels induced by these defects.

The excitations problem has also been approached by the time-dependent(TD) density functional theory formalism. Excellent results have been obtained for finite systems such as atoms, molecules and clusters using LDA or GGA exchange-correlation kernels, as well as for metals. This has not been the case for insulators. The key point is that these functionals miss the long range behavior of the exchange-correlation kernel in semiconductors, and the corrections have been shown to vanish in the thermodynamic limit. It has been clarified that the exchange-correlation functional needs a dependance on the polarization, which determines the long-range behavior of the kernel and thus the response for extended band to band excitations as compared to local approximations based on the electron gas. The exchange-correlation dependence on the polarization is so far unknown. The standard TD-LDA and TD-LSD has been implemented and tests have been performed for localized excitations in the diamond vacancy, in particular the ND1 line observed for the negatively charged vacancy.

Non-collinear magnetism.

The implementation of a non-collinear magnetic moment capability in the major electronic structure codes (LMTO, TB-LMTO, VASP, FLAPW) has been completed. Whereas in the LMTO-codes non-collinearity is implemented in the form of an atomic-sphere-approximation (ASA - fixed quantization axis within each sphere), in VASP and FLAPW the non-collinear version allows to treat the spin-density as a vector-field with a continuous variation of the direction and amplitude of the local magnetic moments. This constitutes a major generalisation compared to the standard electronic structure codes.

Several applications of this new code have been completed. Investigations of non-collinear mag-

netism in ordered intermetallic γ-Fe-Mn compounds and disordered solid solutions have been performed. The striking result is that although canted non-collinear structures are found in the ordered compounds, the structural disorder in the solid solutions induces a collinear ordering of the magnetic moments. Non-collinear spin structures have also been investigated in the closely related Mn-Ni compounds, and current work concerns the investigation of the delicate question of the non-collinear magnetic ground state in α-Mn. Non-collinear spin structures in frustrated triangular antiferromagnetic layers have been investigated, both in the ASA-LMTO and in the unconstrained PAW formalisms, for Mn and Cr monolayers on Cu(111) and for free-standing monolayers. Finally, the formation of helical spin structures has been investigated for Fe/Cr(100) superlattices.

Quasiparticle energies of High T_c superconductors

The quasiparticle spectra of the high T_c superconducting compound $YBa_2Cu_3O_{7-\delta}$ has been calculated from first principles. The calculations are based on the eight-band model developed by Andersen and coworkers to describe the energy bands associated with the CuO_2 bilayers near the Fermi energy, combined with a phenomenological description of the electron-electron attraction. The parameters of the eight-band model were determined by first-principles LDA calculations plus one coupling constant chosen to reproduce the experimentally observed T_c of 92 K at optimal doping. Thus, in the above well-defined sense, the theory is free of adjustable parameters. The new quantities calculated were the two components of the penetration depth tensors λ_a and λ_b, as functions of the temperature T and doping. Three separate points of physical interest are highlighted by the results: Firstly, further evidence has been presented in support of the experimental suggestion that the measured anisotropy of $\lambda_a(0)/\lambda_b(0) \sim 1.5$ implies significant superconducting condensate on the Cu-O chains in the a-b plane. Secondly, it has been shown that the temperature dependence of the superfluid density, as represented by $\lambda_a^2(0)/\lambda_a^2(T)$ and $\lambda_b^2(0)/\lambda_b^2(T)$, is well described by the quasiparticle theory, which also gave a good account of the photoemission experiments. Finally, the calculations reproduced the experimentally observed universality of the $\lambda_\alpha^2(0)/\lambda_\alpha^2(T)$ curves with respect to doping indicating that this dependence, like that of T_c, is in fact governed by the movement of the chemical potential ε_F with respect to a Van Hove singularity in the normal state electronic structure. The dependence on doping of the coherence energy gap has been determined and shown to be BCS-like. Therefore, our results imply that while the normal states of $YBa_2Cu_3O_{7-\delta}$ at various levels of oxygen doping are that of very anomalous metals, their superconducting properties are related to each other as predicted by a simple BCS-like model featuring a nearest-neighbour orbital dependent interaction and realistic energy bands near the Fermi energy ε_F. This suggests that all the electron-electron correlation effects which make the high T_c materials bad metals have gone into the creation of the attractive pairing interaction.

Fully relativistic LAPW codes with molecular dynamics, phonons and optics.

The full potential LAPW codes WIEN99 and FLEUR have been extended with the capabilities of treating the dynamical motion of atoms and spin-orbit interaction. Magnetic anisotropy, magneto-optics and non-collinear magnetism have been studied. In addition, static planar electric fields have been included in the codes, and this has been used to investigate electron densities

and internal strains due to the electric field in GaAs and to interprete synchrotron diffraction measurements. The effect of an applied electric field on the magneto-crystalline anisotropy has been studied and a patent obtained, as this has potentially a large impact on the performance of magnetic recording devices. The calculation of electron-phonon coupling constants in metals has been implemented in the LAPW code. For that purpose, the changes in Hamilton matrix and overlap matrix due to displacements of atoms are necessary ingredients. Two different procedures have been tested: The required quantities have been obtained from (a) two self-consistent calculations, or (b) by use of the linear response method, which had been developed on the basis of the WIEN97 code by the FZJ external team member in Graz before. The results of both methods excellently agree for all test substances and phonon modes. The method is currently applied to study q-dependent electron-phonon coupling constants in superconducting materials.

The code development concerning optical properties in the presence of spin-orbit coupling has been completed in Graz, and the optics package has been updated with magnetooptics now beeing a novel feature in the WIEN97 code.

The efficiency of the FLAPW-method has been improved considerably both by applying advanced parallellization techniques and by choosing a more efficient basis-set, a FLAPW basis-set complemented with local orbitals.

Exchange and Correlation functional for superconductors

The construction of first-principles functionals for the exchange and correlation energy in the superconducting state has made considerable progress. In the first step, a universal LDA-type functional describing the purely electronic correlations in superconductors has been developed. The functional is constructed from the exchange-correlation free-energy density, f_{xc}^{hom}, of a homogeneous electron gas, exposed to an external translationally invariant pairing field. The quantity f_{xc}^{hom}, which is a function of the density and of the induced order parameter, is calculated with many-body perturbation theory by an RPA-type resummation of all normal and anomalous bubble diagrams. In a second step, functionals describing the electron-phonon coupling have been derived. By putting both functionals together and solving the resulting gap equation, we have successfully calculated the critical temperatures of simple metals. The agreement of the calculated T_c's and the experimental numbers, being typically within a few percent, is very encouraging.

The Psi-k2000 Conference

The Psi-k2000 Conference to be held in Schwäbisch Gmünd in August 2000, marks the organisatorial culmination of our network. About 420 people have presently registered for this event, which is almost 50 % more than anticipated. Within the field of electronic structure calculations of materials the Psi-k2000 conference is unmatched worldwide, as also evidenced by the large number of colleagues from America and Japan who are to participate at this conference. The conference will have 19 symposia, of which there will be symposia specializing in each of the subprojects of the present network, with the exception of 'LAPW', which will be covered in the more general 'Band Structure Methods' symposium, and the 'Training and Dissemination' subproject, which does not include research but on the other hand is the main provider of the logistics of the meeting. The meeting will have 4 plenary speakers, 103 invited speakers including

9 from industry, and 111 contributed talks, and 154 posters. All presently employed network post-docs will have contributions at the meeting.

A.2 Joint Patents and Publications

For the list of joint publications, see the full report at:

http://www.ifa.au.dk/~svane/psik-midterm.htm

The complete list of Network publications can be viewed on:

http://www.ifa.au.dk/~svane/psik-publications.htm

PART B - COMPARISON WITH THE PROJECT PROGRAMME

B.1 Research Objectives

The network research comprises atomic-scale computer simulation methodology to understand complex properties and processes in solids and at solid surfaces of a type relevant to industry and basic science. The aim is to develop the methodology of ab-initio computer simulations and to demonstrate its capabilitites to problems of interest to industry. These objectives have certainly been pursued in the research outlined in Section **A.1**, and will continue to be relevant for the remainder of the Network operation.

B.2 Methodological Approach and Work Plan

The methodology employed is that of large-scale 'ab-initio' quantum mechanical computer calculations of properties and processes at the scale of the individual atoms in solids and at solid surfaces. The research is based on the density functional formulation of quantum mechanics, which is implemented in a suite of computer codes, each covering one particular aspect of the problem at hand.

The methodological approach of eight flagship subprojects has not changed. However, one of these, the 'Surfaces' subproject has not been active for the past 12 months. This is due to the movement of Prof. E. Wimmer from the MSI partner to an institution outside the network, after which there has been no scientific leadership of this subproject. Therefore we are presently applying for an enlargement of the network with the inclusion of Prof. Wimmers new affiliation, the Institut Supérieur des Matériaux du Mans (ISMANS), Le Mans, **FR**, as explained in Section **F.1**.

The Table below illustrates the involvement of the Network partners in the different subprojects. It only contains minor changes compared to the work plan of the contract.

B.3 Schedule and Milestones

The work plan, modified under the assumption that the 'Surfaces' subproject will be revived with the inclusion of the ISMANS node to the network, is shown at:

http://www.ifa.au.dk/~svane/work-1.eps

	1 Surfac.	2 f-elect.	3 Interf.	4 Magn.	5 LAPW	6 Excit.'s	7 Supercond.	8 Training
MSI	x		x		x			x
AARHUS		x		x	x	x	x	x
QUB	x		x					x
TUWIEN	x	x		x	x			x
FZJ	x	x	x	x	x			x
HUT				x	x	x		x
UWUERZ		x				x	x	x
CCLRC		x	x			x	x	x

Table 1: Involvement of the Network partners in the Subprojects.

http://www.ifa.au.dk/~svane/work-2.eps

Each subproject is broken down into tasks. The red colour designates tasks which have been essentially completed, blue colour designates tasks, which are being pursued at present, while green colour designates tasks not yet initiated or at a preparatory stage.

Compared to the work plan of the contract, major changes are in the tasks 1A-1D, and 3D. The former is due to the above mentioned temporary halt in the activities of the 'Surfaces' subproject, while the redefinition of task 3D is caused by a change of research focus. After the inauguration of the network it became clear that the metal-titanate interfaces constitute a class of systems of considerable industrial and academic relevance, which are accessible with the methodology developed under the 'Interfaces' subproject. The tasks 4A and 5A, 5B have been completed faster than foreseen, while task 6A has proven more difficult to complete than originally anticipated. Finally, a minor reshuffeling of the workshop program has taken place. The OEP workshop has been turned into a dedicated symposium at the Psi-k2000 conference.

B.4 Research Efforts of the Participants

Participant	Network post-doc		other researchers	
	28 months	48 months	28 months	48 months
AARHUS	10	33	32	54
MSI	9	33	7	40
QUB	27.5	66	69	123
TUWIEN	20.5	33	43	150
FZJ	47	33	58	151
HUT	31.5	33	30	92
UWUERZ	21	33	35	56
CCLRC	0	0	55	43
Total	166.5	264	329	709

Table 2: Total research effort in man months for post-docs financed by the network and for other researchers (for 28 months, and for 48 months according to work plan.)

B.5 Cohesion with Less Favored Regions

The QUB partner in Belfast is a very active partner in the network, being the scientific leader of the 'Interfaces' subproject. Two network post-docs are employed at QUB. On several occasions network funds supported exchange visits to other groups. This partner presented its work in a seminar at the network Industry workshop in Wien, June 1998, and in a Newsletter highlight article also in June 1998, as well as at the Catalysis workshop in May 1999.

B.6 Network Organisation and Management

The Network Management Board (NMB) has the overall responsibility for the coordination and supervision of all activities of the network. The NMB meets twice per year to review the progress in the network program. The board consists of all the scientists-in-charge of the partners, a chairman, a honorary co-chairman, a coordinator, and an external independant representative from industry. The project Coordinator has the responsibility to coordinate and supervise all activities of the Network. In particular he is responsible for coordinating NMB meetings, annual reports and the midterm review. He is also the contact person for outside parties, e.g. other networks and the EU. The scientists-in-charge have the responsibility of the day-to-day management and coordination of the activities within each partner team, in particular the post-doc training. The organisation of training workshops and the newsletter is a dedicated subproject of the network.

The Network maintains a home page:

http://www.ifa.au.dk/~svane/tmr-psik.htm

The Network advertises its workshops, reports and abstracts of papers, vacant positions, scientific highlights etc., in the bi-monthly Psi-k Newsletter:

http://psi-k.dl.ac.uk/psi-k/newsletters.html

Network members contributed to the Psi-k Newsletter six highlights plus one accepted for October 2000:

1. A. Alavi, P. Hu, T. Deutsch, P. L. Silvestrelli and J. Hutter, *Reaction pathway of CO oxidation on Pt(111) from ab initio density functional theory,* Highlights article, Psi-k Newsletter, **27**, 47, June (1998).

2. A. Ayuela, J.-L. Mozos, R. M. Nieminen, and M. J. Puskas, *Nanowires: electronic and ionic structures, cohesive and transport properties*, Highlights article, Psi-k Newsletter **30**, 107 (December, 1998)

3. B. L. Gyorffy, Z. Szotek, W. M. Temmerman, O. K. Andersen, O. Jepsen, G. Litak, A. Martin, J. Annett, K. I. Wysokinsky, *Quasi-particles and Van Hove Scenario for the superconducting Cuprates* Highlights article, Psi-k Newsletter, **33**, 99 (June 1999).

4. E. Wimmer, J.-R. Hill, P. Gravil, and W. Wolf, *Industrial Use of Electronic Structure Methods*, Highlights article, Psi-k Newsletter **34**, 66 (August 1999)

5. A. Svane, W. M. Temmerman, P. Strange, Z. Szotek, and H. Winter, *Self-Interaction Corrected Electronic Structure of Rare Earths* Highlights article, Psi-k Newsletter, **37**, 102 (February 2000).

6. Ph. Kurz, G. Bihlmayer, F. Förster, S. Blügel, L. Nordström, *FLAPW goes non-collinear*, Highlights article, Psi-k Newsletter **38**, 64 (April 2000).

7. D. Hobbs, G. Kresse, and J. Hafner, *Fully unconstrained non-collinear magnetism within the PAW method.*, Highlights article, Psi-k Newsletter, **40**, (October 2000).

The network has organised or co-organised a total of 16 meetings:

1. Industry Workshop: *Electronic Structure Calculations for Industry and Basic Sciences*, Wien, June 1998. 60 attendees, 8 network partners represented.

2. Network Management Board meeting, Wien, June 1998, 10 attendees, 8 network partners represented.

3. Network Management Board meeting, Paris, October 1998, 10 attendees, 8 network partners represented.

4. LAPW mini-Workshop, Jülich, November 1998, 22 attendees, 3 network partners represented.

5. Superconductivity workshop: *The V'th Bristol Workshop on the Boguliubov-de Gennes equations*, Bristol, November 1998, 35 attendees, 2 network partners represented.

6. Topical Workshop: *Materials Under Pressure: From Ices to Metals*, Daresbury, December 1998, 30 attendees, 3 network partners represented.

7. LAPW hands-on workshop, Wien, April 99, 40 attendees, 4 network partners represented.

8. Workshop: *Catalysis from first-principles*, Magleås (Denmark), May 1999, 50 attendees, 4 network partners represented.

9. Topical Workshop: *International Workshop on Orbital and Spin Magnetism of the Actinides,*, Daresbury, June, 1999, 30 attendees, 3 network partners represented.

10. Carr-Parinello hands-on workshop, Trieste, August 99, 80 attendees, 6 network partners represented.

11. Network Management Board meeting, Paris, October 1999, 10 attendees, 7 network partners represented.

12. Psi-k2000 Conference Coordination meeting (Program Committee), Paris, December 1999, 20 attendees, 7 network partners represented.

13. Superconductivity workshop: *The VI'th Bristol Workshop on the Boguliubov-de Gennes equations*, Bristol, April 2000, 44 attendees, 2 network partners represented.

14. FLAPW hands-on Workshop *Full-Potential LAPW Calculations with the WIEN97 Code*, Wien, April 2000, 64 attendees, 4 network partners represented.

15. SIC mini-Workshop: *Electronic Structure and Magnetism in Strongly Correlated Systems*, Daresbury, May 2000, 11 attendees, 2 network partners represented.

16. Discussion meeting: *Catalysis from first principles*, Lyon, July 2000, 46 attendees, 4 network partners represented.

B.7 Connections to Industry

The network partner MSI is an industrial entity, providing software for industry for the simulation of materials properties. This partner is of key importance to the present network providing the link between the academic world of code developers and the potential industrial end users. The MSI partner started as the scientific leader of the 'Surfaces' subproject, but due to a change of staff (see item **F.1** below) it has not felt capable of undertaking that duty any more. The MSI partner remains however an active participant in the network and will continue to work on the 'Surfaces' subproject when it is revived. MSI was one of the main organizers of the Industry workshop in Wien 1998, and a hands-on course on the CASTEP computer code is currently being planned for the autumn 2000. MSI also participated in the LAPW meeting in Jülich 1998, and contributed a highlights article in the Psi-k Newsletter in August, 1999.

Several industrial companies and related entities have participated in the network activities:

1. VDI Technology Center, Association of German Engineers, **DE**
   (S. Mengel, seminar at Industry Workshop, Wien 1998)

2. Siemens Gmbh, Erlangen, **DE**
   (J. Wecker, seminar at Industry Workshop, Wien 1998)

3. Institut Francais du Petrol, Rueil, **FR**
   (H. Toulhoat, seminars at Industry Workshop, Wien 1998, and Catalysis Workshops, Magleås, 1999, and Lyon 2000; P. Raybaud, seminar at Catalysis Workshop, Magleås, 1999)

4. DSM Research, Geleen, **NL**
   (R. Meier, seminar at Industry Workshop, Wien 1998)

5. Haldor Topsøe A/S, Lyngby, **DK**
   (B. Clausen, seminars at Industry Workshop, Wien 1998, and Catalysis Workshop, Magleås, 1999, and Lyon 2000; H. Topsøe, seminar at Catalysis Workshop, Magleås, 1999)

6. Siemens Gmbh, München, **DE**
   (Ch. Werner, seminar at Industry Workshop, Wien 1998)

7. TOTAL Raffinage et Distribution, Harfleur, **FR**
   (F. Hutschka, seminar at Industry Workshop, Wien 1998)

8. Okmetic Ltd., Espoo, **FI**
   (O. Anttila, seminar at Industry Workshop, Wien 1998. Frequent information exchanges with HUT network partner (semiconductor processing).)

9. BASF AG, Ludwigshafen, **DE**
   (P. Erk, seminar at Industry Workshop, Wien 1998)

10. OSRAM, Schwabmünchen, **DE**
    (J. Almanstötter, attending FLAPW Hands-on course, Wien 2000)

11. Ford Motor Company, Dearborn, Michigan, USA
    (A. Bogicevic, seminar at Catalysis workshop, Lyon 2000)

12. Motorola, Tempe, Arizona, USA
    (R. Ramprasad, seminar at Catalysis workshop, Lyon 2000)

13. Petroleos de Venezuela, Caracas, Venezuela,
    (M. E. Grillo, seminar at Catalysis workshop, Lyon 2000)

14. Lubrizol, Wickcliffe, Ohio, USA
    (A. Chaka, seminars at Catalysis workshops in Magleås, 1999, and Lyon 2000)

15. Coherent Tutcore Inc., Tampere, **FI**
    (frequent information exchanges with HUT partner (nitride semiconductors).)

The Industry Workshop held in Wien, 1998, has developed into an annual event with the Catalysis workshops in Magleås, 1999, and in Lyon, July 2000. These workshops are organised in collaboration with the ESF STRUC programme. For the Psik2000 conference in August 2000, 9 industrial speakers are invited. Though we do not want to exaggerate the impact of our methodology on the industrial production of goods at the present time, one certainly sees a growing interest in our achievements and a number of growth points and new initiatives in the field.

PART C - TRAINING

C.1 Employment of Young Researchers

The young researchers employment program is displayed in Table 2 on page 13. No pre-doc's have been employed, nor have they been foreseen in the contract. A total of 166.5 man months of post-doc training has been financed, to be compared with the contract deliverable of 264 man-months for the entire network period.

By extrapolating the above numbers to the end of the contract, we conclude that we can exceed the number of man-months of training stated in the contract.

C.2 Training Programme

The day-to-day training of the post-docs is provided by the scientist-in-charge and other research staff of the network partner hosting the post-doc. The hands-on training workshops (3 have been held up to now, with a total of 184 participants) provide an intensive training environment

for young researchers. Typically these courses last a week, with mornings devoted to lectures and excersises in the background theory, while afternoons concentrate on the practical use of a particular computer code. Topical workshops likewise facilitate the information exchange and broadening of the general scientific perspective of young researchers. Finally, individual secondments to other research groups of a duration of between 1 week and several months finance the more specialized training in techniques outside the experience of the hosting institution.

C.3 Factual Information on the Young Researchers

Name	Nationality	Age	Start Date	End Date	Speciality
José Luis De Los Mozos Liz	**ES**	32	1/5/98	31/12/00	P-10, P-11
Peter Gravil	**GB**	30	1/6/98	28/2/99	P-10, P-13
Gustav Bihlmayer	**AT**	32	1/9/98	31/8/00	P-10
Lars Fast	**SE**	33	1/10/98	30/9/00	P-10
David Hobbs	**IE**	28	15/10/98	14/10/00	P-10
Sean Clarke	**GB**	25	1/11/98	31/10/00	P-10
Barbara Montanari	**IT**	29	1/2/99	31/1/01	P-10
Arnaud Marmier	**FR**	28	15/8/99	14/8/01	P-10
Leon Petit	**LU**	35	1/9/99	28/2/02	P-10
Jason James Hogan-O'Neill	**GB**	26	15/1/00	31/12/01	P-10
Georg Madsen	**DK**	28	1/2/00	31/01/01	P-10, C-24, C-25

Table 3: List of Young Researchers. All are post-doc's.

.

Name	Place of work	Country	Prev. with other partner
José Luis De Los Mozos Liz	Helsinki University of Technology	**FI**	no
Peter Gravil	Molecular Similations s.a.r.l., Orsay	**FR**	no
Gustav Bihlmayer	Research Center Jülich	**DE**	no
Lars Fast	University of Würzburg	**DE**	no
David Hobbs	Vienna University of Technology	**AT**	no
Sean Clarke	Research Center Jülich	**DE**	no
Barbara Montanari	Queen's University of Belfast	**GB**	FZJ
Arnaud Marmier	Queen's University of Belfast	**GB**	no
Leon Petit	University of Århus	**DK**	no
Jason James Hogan-O'Neill	Helsinki University of Technology	**FI**	no
Georg Madsen	Vienna University of Technology	**AT**	AARHUS

Table 4: Working place of Young Researchers.

PART D - SKETCHES OF THE YOUNG RESEARCHERS

D.1

At present 10 young researchers are employed under the network contract. Each of them give a short presentation of themselves, see the full report:

http://www.ifa.au.dk/~svane/psik-midterm.htm

PART E - NETWORK FINANCING

E.1

Partner	Expenditure	Budget	Percentage
AARHUS	62096	161600	38 %
MSI	43736	176400	25 %
QUB	94657	218500	43 %
TUWIEN	75972	176400	43 %
FZJ	105578	197600	53 %
HUT	74298	176400	42 %
UWUERZ	61307	191000	32 %
CCLRC	54185	188100	29 %
Total	571829	1486000	38 %

Table 5: Expenditure of each partner (Euro), compared to budget. The reporting period (28 months) constitutes 58 % of the total Network duration.

A	B	C	D	Total
416125	87140	1880	66684	571829
73 %	15 %	0 %	12 %	100 %

Table 6: Break down of total expenditure into cost categories A (personnel), B (networking), C(other direct costs), and D(overheads).

The network has till now spent 38 % of its funds. In the beginning we encountered difficulties in recruiting post-docs, and the spending the first year was only 10 % of the contract sum. The spending increased to 20 % in the second year, and we estimate the third year to exceed 30 %. Therefore, with the present level of spending we anticipate to use up all network funds within the network duration.

PART F - PROPOSED REVISION TO THE CONTRACT

F.1

The 'Surfaces' subproject has not been active for the past 12 months. This situation is caused by the movement of the former MSI scientist-in-charge Prof. E. Wimmer from MSI to an institution outside the network, the Institut Supérieur des Matériaux du Mans (ISMANS), Le

Mans, **FR**. Since then, there has been no person at MSI feeling capable of taking over the scientific leadership of this subproject. Therefore, we are presently applying for an enlargement of the network with the inclusion of Prof. Wimmers new affiliation at ISMANS. (Application dated May 9, 2000).

Another scientist-in-charge, Prof. J. Hafner, has moved his chair form the Technical University of Wien (the TUWIEN partner) to the University of Wien (UNIWIEN). He maintains a lectureship at the TUWIEN, but this is a temporary arrangement. We would like to keep Prof. Hafner in the network, in particular as the scientific (and financial) leader of the 'Magnetism' subproject. Therefore, we will soon send in an application for a network change such that the TUWIEN partner be replaced by UNIWIEN as a network partner. UNIWIEN is presently an external team member of our network, due to collaborations with other researchers at this institution. We would like TUWIEN to remain an external team member for similar reasons.

6 News from the ESF Programme

"Electronic Structure Calculations for Elucidating the Complex Atomistic Behaviour of Solids and Surfaces"

6.1 Reports on Collaborative Visits

Report on collaborative visit of Carme Rovira (University of Barcelona) to Max-Planck-Institute Stuttgart

August 26 - September 6, 2000

First principles modeling of hemeproteins and coenzymes

I visited the group of Michele Parrinello (Max-Planck-Institut fuer Festkoerperforschung, Stuttgart) during the period Aug. 26 - Sept. 6. The purpose of the visit was to discuss about our collaboration on hemeprotein modeling. In particular, on the application of the new QM/MM schemes developed in the group of M. Parrinello (Eichinger et al. JCP 1999) to the study of several processes related with the binding of ligands to myoglobin.

Up to now we have studied the influence of the distal pocket conformation on the structure and vibrational properties of the heme-ligand bond. We found that the structure remains practically unchanged with respect to simple heme models (J. Phys. Chem. A, 101, 8914, 1997; Chem. Eur. J., 5, 250, 1999; Biophys. J., 78, 93, 2000) but there are significant changes in the ligand vibrations. Our main concern in this study has been how to select appropriate protein structures as starting ones for the QM/MM calculations. These structures were taken from previous classical simulations with the same force-field (J. Am. Chem. Soc., 121, 6444, 1999) aimed to identify the main conformational substates.

The results we have up to now can explain several controversial features of the infrared spectra of ligated myoglobin. In view of the good results obtained with this approach and the rapid development of techniques to accelerate dynamic processes in proteins, it will be possible in the near future to tackle other problems of interest such as the mechanism ligand entry and escape from the heme pocket.

Apart of our work on heme proteins, we also discussed on the modeling of the mechanism of action of the B_{12} coenzyme. An analysis of the structure-energy- spin relations of its inner cobalt-corrin ring will appear soon (Rovira, Kunc, Hutter, Parrinello, Inorg. Chem.).

Overall the visit was very fruitful and I acknowledge the Ψ_k network for making it possible.

Carme Rovira

6.2 Reports on Workshops/Conferences

6.2.1 Report on CECAM Meeting

Report on the discussion meeting "Catalysis from First Principles"

The objective of the meeting (held in Lyon at CECAM, from July 5 to 8, 2000) was to review the status of total-energy calculations as a basis for modeling and understanding of chemical reactions on solid surfaces. A strong focus was placed on the prospects of calculational methods becoming a tool in the design of new catalysts. An additional objective was to bring together researchers from the electronic structure and molecular-dynamics communities as well experimental surface-science and catalysis researchers from academia and industry.

The format of the workshop was a small meeting (about 40 participants), in the approximate ratio theory/experiment/industry=2/1/1. There were review talks, short presentations and ample time for discussion including short (one overhead) contributions on specific topics. Also a poster session was organized.

The meeting's web page

http://www.fhi-berlin.mpg.de/th/Meetings/Lyon2000/Lyon-1.html

provides the possibility to download the workshop program, abstracts of talks and posters, and a list of participants (with full addresses).

I like to thank again the host institute, to be specific, Michel Mareschal and Emmanuelle Crespeau at CECAM for their competent, efficient, and friendly help. I personally enjoyed the meeting and felt that it was successful.

The following report was written by Dr. Anne Chaka (The Lubrizol Corporation) and Dr. Alexander Bogicevic (Ford) and summarizes their personal impression.

Berlin-Dahlem, September 11, 2000
Matthias Scheffler

Personal notes from participants:

The discussion meeting on "Catalysis from First Principles", held in Lyon, France, was founded on contributions from 46 participating scientists from 12 different countries worldwide. A healthy division between theorists and experimentalists from both academia and industry formed a very fertile ground for information exchange and intense, yet cordial, discussions and debates. The wide range of approaches and methodologies was impressive, including atomistic design to purely empirical combinatorial and parallel approaches. All came with a common goal in mind: to

improve on existing technologies and pave the road for the development of the next generation of catalysts.

This type of broad, inclusive meeting on a focused topic combines many of the best features of both large-scale conferences and smaller, more specialized workshops. It achieves several noteworthy goals:

(i) Bringing together researchers from around the world and putting them in a close environment for dynamic scientific exchange.

(ii) Allowing for critical comparisons to be made between similar methodologies, so that one can return with a sense of the quality of one's own research.

(iii) Mixing people from quite different backgrounds, i.e. industry and academia, experiment and theory, and serving to pinpoint existing gaps between science and technology as well as ways to overcome them. There is synergy to be gained by applying different methods to the same problem, as one method may be more appropriate to answer one aspect of a problem than another, yet together they provide a more complete and clear picture of complex phenomena.

(iv) Providing a very nice and comfortable forum for graduate students looking to learn about and make contact with industrial representatives.

It is clear that all of these accomplishments stand or fall with the intricate balance of attendees and the structure of the meeting, and the organizers achieved this in a very impressive way.

A consistent theme throughout the meeting was how to address the gap between fundamental and applied heterogeneous catalysis. Specifically, discussions revolved around how to link clean UHV experimental and theoretical work to real-world catalytic conditions with much higher pressures and greater materials complexity. As a very interesting and eye-opening example, Robert Schlögl (Berlin, Germany) nicely illustrated the question of "how essential is complexity" in his presentation on how Fe_2O_3 catalyzes the dehydrogenation of ethyl benzene to form styrene in commercial processes. Theoretical and UHV experimental studies have historically focused on alpha-Fe_2O_3, establishing which surface is the most stable in equilibrium with oxygen at different partial pressures in the environment (Wang, et al.), how ethyl benzene is adsorbed (Weiss, et al.), and what the fundamental steps of dehydrogenation consist of on a clean $Fe_2O_3(0001)$ surface. Yet the most recent results from Robert Schlögl's group indicated that the rate of dehydrogenation actually **increases** after the catalytic surface is covered with carbon. Further investigation revealed that it is the formation of oxygenated polynuclear aromatic species on the surface, formed from the polymerization and subsequent graphitization of styrene on the surface, which were primarily responsible for activity in the commercial catalyst. To test this hypothesis, carbon nanotubes were synthesized and oxygenated, and found to have very high catalytic activity, in the total absence of iron oxide! Hence the iron oxide is important for the initial stages of styrene formation and subsequent graphitization, but is not the primary active species for the majority of the life of the commercial catalyst. This type of insight would not be possible from clean, over-simplified model experiments or calculations, and underscores the

importance of bridging the pressure and materials gap and studying a reaction system in its full complexity.

The presentations of the latest experimental results highlighted the incredible degree of resolution in time and space that is now possible with current techniques. For example, Martin Wolf (Berlin, Germany) showed how femtosecond laser spectroscopy allows the distinction between electron and phonon mediated chemical reactions on a surface. Using STM, Flemming Besenbacher (Aarhus, Denmark) very graphically illustrated how promoter atoms like Co perturb the morphology of MoS_2 nanoclusters used as a model system for commercial hydrodesulfurization catalysts. In addition, a novel STM system, capable of operating at 1 bar, clearly showed that a Cu(110) surface responds the same to hydrogen whether under UHV or atmospheric pressure. Another key theme at the meeting was the importance of integrating theory and experiment. For complex systems, theory can provide the details of atomic structure and reactivity to aid in the interpretation of ambiguous spectra, the results of macroscopic experiments and aid in understanding reactivity at defects or within zeolites, which is difficult to probe experimentally. In the case of nanotechnology where smaller particles behave qualitatively different than their macroscopic counterparts, theory can be extremely valuable in sorting out whether this is due to electronic effects or perhaps just bringing reactants into close proximity (Uzi Landman, Atlanta, Georgia). New combinatorial approaches to catalytic design also require greater understanding and descriptors which can be obtained via theory. As Ferdi Schüth (Mühlheim, Germany) demonstrated, "Combinatorial chemistry does not mean replacing one stupid experiment with a thousand."

It is not possible in this article to mention all of the new, excellent work which was presented and discussed at the meeting. But as two of the industrial participants, we have no hesitation in stating that we found this meeting to be extremely valuable for our work for both the content and the contacts.

Anne M. Chaka
The Lubrizol Corporation
Ohio, U.S.A.

Alexander Bogicevic
Ford Research Laboratory
Michigan, U.S.A.

6.2.2 Report on CECAM "Excited states" workshop

CECAM WORKSHOP "EXCITED STATES AND ELECTRONIC SPECTRA"

Sponsored by CECAM and by the European Science Foundation Programme "Electronic Structure Calculations for Elucidating the Complex Atomistic Behaviour of Solids and Surfaces" (Psi-k)

Organised by **Lucia Reining**, Ecole Polytechnique, France
Giovanni Onida, University "Tor Vergata", Rome, Italy
Angel Rubio, University of Valladolid, Spain

The workshop was concerned with *ab initio* calculations of excited electronic states, and related spectroscopic properties, in condensed matter applications as well as atomic and molecular physics (nanostructured materials). Our aim was to bring together researchers of different backgrounds: density functional, many-body, and nuclear physics and quantum chemists' approaches in order to assess the present status of the ab-initio computation of electronic excitation spectra, and in order to strengthen the growing exchange and merging of the traditionally different communities.

In fact, the workshop has shown to continue an important tendency which has grown out of the previous workshops of this series ("Excited electrons in Molecules, Solids and Atoms", CECAM (Lyon), 1997; "Spectroscopy of electronic excitations in materials" in Valladolid (Spain), 1998 ; "Excited states and electronic spectra", CECAM (Lyon), 1999): there is a strong interest from an increasing community - again, the number of participants has been considerably bigger than the number of invited speakers. In spite of the relatively large audience (about 50 participants, of which 22 speakers), discussions were lively and not restricted to a limited group of people, as one could have feared in this situation.

It has also been very important that a big number of PhD students and post docs could participate, thanks to the financial support of ESF/Psi-k.

The program and the discussions have been centered around several main questions:

a) One-particle excitations: Calculation of band structures and lifetimes, dependence of the GW approach on the "starting point" (LDA, Hartree-Fock...), self-consistency.

b) Use of many-body theory for the calculation of total energy.

c) Calculation of two-particle excitations: solution of the Bethe-Salpeter equation, optical properties, loss function. There is a increasing number of applications of the *ab initio* Bethe-Salpeter method, including complex systems (like surfaces) and different spectroscopies (like electron energy loss).

d) Theoretical and practical questions: problems of self-consistency, vertex corrections, correlation functionals, description of superconductivity. And pseudopotential versus all electron calculations - this point has yielded lively discussions, but no definitive conclusion!

e) Applications centered in the field of nanostructures: even relatively complex structures, close to reality, are today accessible to a sophisticated (even though still approximate) description.

f) Comparison of TDDFT (Time-dependent density functional) and Green's functions approaches for the calculation of excited states properties. TDDFT in the adiabatic LDA approximation has turned out to be successful in small systems. A detailed explanation of this success, and its unsuccess in infinite systems, is still missing. This is litterarily the same conclusion as for last year's workshop: we'll have to work on that!

The detailed program, and the abstracts, are attached below.

Programme

Thursday 20 July		
09:00	Welcome and Announcements	
Chairperson: C.O. Almbladh		
09:10	Introduction (U. von Barth)	
09:20	W.C. Mackrodt	A simple direct approach to the calculation of the excited states of NiO based on HF and DF theory
09:55	M.D. Kuzmin	Quasi-Particle Band Structure and Dielectric Eigenpotentials of Diamond
10:30	A. Schindlmayr	Decay properties of the one-particle Green function in real space and imaginary time
10:55	Coffee Break	
11:20	P.G. Gonzalez	Accuracy of many body perturbation theory for calculating ground

		state properties
11:45	P. Friera	Total energy calculations from self-energy models
12:10	B. Holm	Total energy from the Galitskii-Migdal formula using realistic spectral functions
12:30	Lunch	

Chairperson: A. Rubio

14:20		
14:30	F. Bechstedt	Calculation of optical properties for systems with large supercells
15:05	G.M. Rignanese	Quasiparticle band structure of C2H4 adsorbed on the Si(001)-2x1 surface within the GW approximation
15:25	J.M. Pacheco	Magnetic LEGO structures
15:45	Coffee Break	
16:10	J.M. Pitarke	Electron and hole dynamics in simple and noble metals
16:45	W. Eckardt	The lifetime of hot electrons inm metals determined by timeresolved two-photon-photoemission(TR2PPE): The role of

		transport-effects, d-band catastrophy, and transient excitons.
17:20	Break	
17:35	ROUND TABLE 1 (Coordinator: Rex Godby)	

Friday 21 July

09:00	Introduction (C.O. Almbladh)	

Chairperson: O.Gunnarson

09:10	A. Eguiluz	Calculations of electronic excitations in metals within TDDFT: Do we know how to handle correlation yet?
09:45	J.F. Dobson	STLS approach for inhomogeneous systems
10:20	Coffee Break	
10:45	T. Kreibich	Multicomponent Density-Functional Theory for Molecules in Strong Laser Pulses
11:20	V. Olevano	Excitonic effects in EELS spectra of semiconductors
11:55	M. Rohlfing	Structural relaxation in excited states
12:30	Lunch	

Chairperson: G. Onida

		The Baym-Kadanoff method and its all-electron

14:30	A. Eguiluz	implementation for semiconductors: What does it take to do a good calculation of the band gap?
14:50	5' introductions to posters, part 1	
15:25	Coffee Break	
15:40	5' introductions to posters, part 2	
16:15	ROUND TABLE 2 (Coordinator: L. Reining)	
17:15 - 19:15	POSTER SESSION	
20:00	SOCIAL DINNER	

Saturday 22 July

Chairperson: J. Dobson

09:00		
09:10	O. Gunnarson	Core-level line shapes of cuprates: Effects of valence and of Cu-O network
09:45	A. Marini	Plane-waves DFT-LDA calculation of the electronic structure and absorption spectrum of Cu
10:05	Coffee Break	
10:30	E. Molinari	Linear and non linear optical properties of semiconductor quantum wires and dots
11:05	A. Ruini	Optical Properties of Semiconducting Conjugated Polymers: a First-Principles Study

11:25	C. Delerue	Excitonic and quasiparticle gaps in Si nanocrystals
12:00	Concluding Remarks (Rex Godby)	
13:00	End of the Cecam Workshop	
15:00	Internal Meeting of the NANOPHASE groups	
18:00	End	

Abstracts of Talks

Calculation of optical properties for systems with large supercells

F. Bechstedt(1), B. Adolph(2), G. Cappellini(3), J. Furthmueller(1), and H.-Ch. Weissker(1)
(1)Friedrich-Schiller-Universitaet, Max-Wien-Platz 1, 07743 Jena Germany
(2)University of Toronto
(3)Universita' di Cagliari

Abstract

Si and Ge nanocrystals embedded in a wide-gap semiconductor like α-SiC are potentially interesting systems for possible electroluminescence applications. A theoretical understanding of these systems is yet to be achieved, both for the optical properties under inclusion of the relevant many-body effects and for the structural and electronic properties. We present first attempts to describe these properties using parameter-free electronic structure calculations and large supercells. A plane-wave-pseudopotential code (VASP) is used to calculate the electronic structure within density-functional theory (DFT) in local-density approximation (LDA). Ultrasoft non-normconserving pseudopotentials allow the *ab-initio* treatment of supercells with up to 512 atoms, even in the case of first-row elements. Each supercell contains one cluster, the remaining space is filled with matrix material. The maximum dot diameters are about 1 nm. Examples are mainly structures made of group-IV materials. In the present talk we focus our attention on three main problems.

- The problem of wave-function augmentation for non-normconserving pseudopotentials is solved by constructing all-electron wave functions using Blöchl's projector-augmented

wave (PAW) method [1]. As an advantage nonlocal contributions to the optical matrix elements do not occur. Spectra are compared with those obtained using normconserving pseudopotentials and the FLAPW method.

- The huge supercell size drastically restricts the number of k-points. Nevertheless we prefer to use the tetrahedron method for the optical calculations. Unfortunately the increase of the supercell size gives rise to many band crossings which prevent the identification of the same band at the tetrahedron vertices. We present a highly efficient and robust extrapolative Brillouin-zone integration scheme based on second-order $k \cdot p$ perturbation theory (cf. [2]).
- We use the simplified treatment of the GW self-energy developed by Cappellini et al. [3] in the beginning of the 90's to calculate the quasiparticle corrections for supercells with several hundreds of atoms . The dielectric constant and the electron density determining the RPA screening are obtained within DFT-LDA. Despite the complications with the augmentation of the Bloch integrals we show agreement with calculations using two-atom cells. Computations for embedded clusters are in progress.

[1] P.E. Blöchl, Phys. Rev. B**50**, 17953 (1994)

[2] C.J. Pickard and M.C. Paine, Phys. Rev. B**59**, 4685 (1999)

[3] F. Bechstedt, R. Del Sole, G. Cappellini, and L. Reining, Solid State Commun. **84**, 765 (1992); G. Cappellini, R. Del Sole, L. Reining, and F. Bechstedt, Phys. Rev. B**47**, 9892 (1993)

Excitonic and quasiparticle gaps in Si nanocrystals

C. Delerue, M. Lannoo and G. Allan

IEMN, Dept. ISEN 41 boulevard Vauban, 59046 Lille Cedex, France

Abstract

One of the most challenging problems concerning semiconductor nanocrystals remains the accurate prediction of their excitonic energy gap. For silicon, a number of calculations of the independent particle gap have been performed based either on empirical techniques (tight binding [1] or pseudopotentials [2]) or on the ab initio local density approximation (LDA) [3]. In the latter case, as LDA underestimates the bulk bandgap, the results are usually shifted by the bulk correction. Interestingly these corrected LDA bandgaps are in quite good agreement with the best tight binding or pseudopotential results [3,4]. The second step has usually been to substract from this value the screened direct electron-hole attraction. However the whole procedure is not clearly justified and conflicting points of view [5-7] have been expressed concerning its validity. The aim of this work is thus to clarify this problem. We present calculations of the one and two particle excitations in silicon nanocrystals. The one-particle properties are handled in the GW approximation and the excitonic gap is obtained from the Bethe-Salpeter equation. We develop a tight binding version of these methods to treat clusters up to 275 atoms. The self-energy and Coulomb corrections almost exactly cancel each other for crystallites with radius larger than 0.6 nm. The result of this cancellation is that one-particle calculations give quite accurate values for the excitonic gap of crystallites in the most studied range of sizes. We also show that the self-energy and Coulomb corrections are dominated to a large extent by classical electrostatic contributions.

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STLS approach for inhomogeneous systems

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Abstract

The interacting density-density response function of an inhomogeneous electronic system has poles at frequencies equal to exact excitation energies. In time dependent density functional theory (TDDFT), all aspects of the response beyond the RPA are described by the exchange-correlation kernel f_{xc}, or equivalently the dynamic local field factor G. This quantity is in general spatially and temporally nonlocal, but early TDDFT calculations assumed f_{xc} to be local in both domains. Numerical experimentation suggests that the temporal locality assumption is surprisingly good in many systems, so that it is worthwhile to consider spatial nonlocality alone. The Singwi-Tosi-Land-Sjolander (STLS) approach represents an attempt to find an optimal spatially nonlocal field factor, based on a heuristic factorization of the dynamic pair distribution. It has the unique feature that the static pair distribution is selfconsistently determined in the process. This approach is rather successful for correlation energies and plasmon properties of weakly to moderately correlated uniform electron gases. It apparently has not so far been applied to nonuniform gases, presumably because of the increased computational complexity. Recent work on the full RPA description of inhomogeneous systems suggests that the STLS scheme is now well within computational reach, at least for geometrically simple inhomogeneous systems such as jellium surfaces and atoms. The STLS theory does require some modification for inhomogeneous systems, and some aspects of this problem will be discussed.

Total energy calculations from self-energy models

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Abstract

In the framework of Many-Body Perturbation Theory (MBPT), the total energy of a system of interacting electrons can be calculated via the Galitskii-Migdal formula. This requires an accurate knowledge of the one-particle Green's function of the system in a very long range of frequencies. The Green's function can be calculated within the self-consistent *GW* approximation, which has led to accurate total energies when applied to homogeneous electron gases [1,2]. However this approach is computationally very expensive and at the moment its application to complex systems of industrial interest is not feasible.

We propose a model, based on self-consistent *GW* results for the homogeneous electron gas, which contains an accurate description of the non-locality and frequency-dependence of the self-energy. This model allows one to calculate total energies without significantly increasing the numerical cost of standard density-functional theory calculations, thus making it useful for applications to large systems. The method has been tested against accurate quantum Monte Carlo results for the linear response of the homogeneous electron gas and structural properties of bulk silicon.

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Accuracy of many body perturbation theory for calculating ground state properties

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Abstract

or the last thirty years, Density Functional Theory (DFT) has been the standard for obtaining the ground-state properties of many-electron systems. However, the increasing computational speed and capacity allow the study of a growing number of complex systems using DFT. Although in many cases amazing new results have been obtained (specially when complemented with molecular-dynamics), there are more and more situations where the limitations of the standard approximations in DFT are evident. On the other hand there is a number of exact formal properties that such common implementations of the DFT fail to fulfil. The main problem is that, being DFT an exact theory, it relays on the description of many-body effects (that are highly non-local) by means of a local potential. Generalizations of the DFT allowing the use of non-local potentials have been recently proposed, but some fundamental tests (like the description of the linear response in the homogeneous limit) seem to be too sensitive to the details of the functionals so developed.

Green's function many body perturbation theories (like Hedin's GW approximation) can provide a different way to overcome the limitations of present DFT. In the GW the non-local effects are taken directly into account, and the Coulomb interaction is dynamically screened. Both things are done in a closed way, without the resort of additional models albeit those inherent to the GW theory itself. Moreover, the interacting Green's function G is the final output of any GW calculation and the knowledge of G is enough to determine many ground-state properties, including the electron density and the total energy.

The above comments suggest that GW approximation might be a very valuable way for determining ground-state properties, but such hypothesis has to be confirmed with actual implementations of the theory. So far, the performance of GW in these types of calculations

has been only tested in some model system and in the homogeneous electron gas (HEG) in the range of metallic densities. In this work we present GW results for the ground-state of HEG, covering a broad range of densities in both spin-unpolarized and fully spin-polarized phases.[1] Other issues, such as conservation of the number of particles and possible implications in the development of simpler models to calculate total energies will be also discussed.

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Core-level line shapes of cuprates: Effects of valence and of Cu-O network

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Abstract

We calculate the charge density of mono-, di- and trivalent Cu compounds, and demonstrate that the difference in the net Cu charge is very much smaller than the formal valence would suggest.

The chemical shift nevertheless behaves in the expected way, with the strongest core-level binding energy for the trivalent compound.

We then focus on the shape of the core-level spectrum, and show that there is a large difference between the mono- and divalent compounds and a less pronounced difference between di- and trivalent compounds. For the divalent compounds the dependence of the spectrum on the Cu-O network is studied extensively. Although the core spectrum is usually considered as a local probe, the line shape depends rather sensitively on the coupling Cu-O-Cu to the second nearest neighbor (Cu) sites. We show that this behavior can be rather well reproduced in the Anderson impurity model. The reason for the dependence on the Cu-O network is analyzed.

Multicomponent Density-Functional Theory for Molecules in Strong Laser Pulses

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Abstract

Owing to the rapid developments in laser technology, ultra-short high-intensity laser pulses have become available in recent years. Considering the interaction of such extreme

radiation fields with matter, one observes a wealth of exciting new phenomena which cannot be explained by ordinary perturbation theory.

A consistent ab-initio approach to the strong-field dynamics of atomic or molecular systems should thus allow for a non-perturbative treatment of the external radiation field as well as for an appropriate description of the quantum behavior of the electronic and nuclear degrees of freedom involved. For that purpose, we propose a *time-dependent multicomponent density-functional* approach to molecules in intense laser pulses. It is shown that this method provides a numerically efficient way to calculate the strongly non-linear dynamics of an interacting many-particle system.

After an overview over the fundamental theorems, we investigate approximations for the time-dependent effective potentials which, in particular, contain the exchange-correlation effects of the system. The method is then used to discuss the strong-field behavior of a simple model system.

Comparisons to exact solutions allow us to assess the quality of the approximations employed within the proposed multicomponent density-functional scheme.

A simple direct approach to the calculation of the excited states of NiO based on HF and DF theory

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Abstract

NiO is a paradigm magnetic oxide whose properties have been studied extensively for many years. There now exist good optical, EELS and other data on the low energy excitations in the range 1 - 5 eV for stoichiometric NiO, and, importantly, also for LixNi1-xO, on the basis of which theory and computation can be assessed. In this talk I will first summarise this data and draw certain conclusions which have suggested(forced?)a direct approach to the calculation of the local d-d excited states both for the bulk and (100) surface [1,2]. I will then consider the strong optical absorption at 4 eV in relation to the band gap, (I+A) and charge-transfer excitations, based on both HF and KS approaches and consider, briefly, the contribution of electron correlation to these quantities.

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Total energy from the Galitskii-Migdal formula using realistic spectral functions

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Abstract

Although many body perturbation theory (MBPT) for quite some time has been used to determine quasiparticle energies and optical properties of solids, traditionally the issue of ground state energy has not been addressed with this method. Rather, most efforts in that direction have been concentrating on various mean field theories. The success of density functional theory (DFT) has enhanced this evolution. However, there are certain systems for which known approximations for the so called exchange-correlation potential within DFT cannot correctly reproduce the observed ground states or the calculated groundstate properties deviate significantly from experiment. In situations like these, an alternative is to have a theory that does not depend on such approximations, but rather is derived from first principles within MBPT, albeit with some other form of approximation. We here investigate two such schemes, rather closely related to each other, in order to highlight the essential properties of a MBPT that correctly describes spectral properties *and* ground state energies. As a first step, we have investigated the case of the electron gas which provides a starting point for more general cases of real materials.

Electron and hole dynamics in simple and noble metals

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Abstract

We present a detailed analysis of electron and hole dynamics in simple (Al) and noble (Cu, Ag, and Au) metals, by means of first-principles many-body calculations. Quasiparticle damping rates are evaluated from the knowledge of the electron self-energy, which we compute within the GW approximation of many-body theory. Inelastic lifetimes are then obtained along various directions of the electron wave vector, with full inclusion of the band structure of the solid. Average lifetimes are also reported, as a function of the electron energy. In Al, splitting of the band structure over the Fermi level yields electron lietimes that are smaller than those of electrons in a free-electron gas. In the noble metals, a major contribution from d electrons participating in the screening of electron-electron interactions yields electron lifetimes that are above those of electrons in a free-electron gas with the electron density equal to that of valence electrons. While holes in a free-electron gas are known to live shorter than electrons with the same excitation energy, our results indicate that d-holes in noble metals exhibit longer inelastic lifetimes than excited sp-electrons, in agreement with experiment.

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Quasiparticle band structure of C2H4 adsorbed on the Si(001)-2x1 surface within the GW approximation

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Abstract

Adsorption of molecules on silicon surfaces is a very active research field. This interest is motivated by their technological importance in microelectronic device manufacturing, but also by the fundamental interest on the interaction of molecules with the dangling bond states of semiconductor surfaces. One typical example is the adsorption of the ethylene (C_2H_4) molecule on the Si(001) surface which is particularly important for diamond film growth, and formation of silicon carbide on crystalline silicon.

In a very recent angle-resolved photoemission study of C_2H_4 on single-domain Si(001)-2×1 using synchrotron radiation, the electronic structure of the adsorption system has been investigated in detail [1] allowing to identify seven ethylene-derived peaks. Two of these states, $1b_{3u}$ and $1b_{2g}$, were found to delocalize along the Si-Si dimer rows while they are localized in the direction perpendicular to the rows. In connection with this study, a calculation of the electronic structure has also been carried out [2] within the local-density approximation (LDA) to DFT showing a qualitative agreement with experiment: the 1D-dispersion features of the $1b_{3u}$ and $1b_{2g}$ states are well-reproduced. But, *the absolute energies of the adsorbate states are systematically shifted up with respect to the substrate states.*

By performing a careful analysis of the STM images obtained for various coverages of the C_2H_4/Si(001) surface [3], it was found that the C_2H_4 molecules appear slightly darker than the bare silicon dimers when tunneling out of the surface (i.e. the STM tip moves lower in order to maintain the same tunneling current). This can only be understood in terms of electronic structure effects. Following up this study, STM images were computed within DFT-LDA for a semi-covered surface [4]. In clear contradiction with experiments, the isolated molecules were found to appear brighter than the bare dimers. However, the experimental contrast could be recovered by taking into account the influence of the tip-induced electric field.

The theoretical studies mentioned above [2,4] rely on the electronic band structure obtained within the DFT. However, there is no formal relation between the Kohn-Sham eigenvalues and the electron excitation spectra, which can therefore can be significantly different. In this work, we present a study of the electronic properties of the C_2H_4/Si(001) surface using an accurate many-body formalism within a quasiparticle approach. The calculations are performed within the *GW* approximation [5] which has been shown to yield quasiparticle energies within 0.1-0.2 eV as compared to photoemission experimental data for bulk crystals [6] and surfaces [7]. Here, for the first time to our knowledge, we investigate the capability of the *GW* approximation to describe the electronic energy levels of molecular adsorbates on semiconductor surfaces.

On the one hand, we investigate the fully-covered surface. We show that the quasiparticle band structure is in an excellent agreement with photoemission spectra. The self-energy corrections for the adsorbate states are found to be about 1.5 eV larger than those for the

bulk states, demonstrating the dependence of the self-energy correction on the localization of the wavefunctions. On the other hand, we also consider the semi-covered surface. By extrapolating the self-energy correction taking the localization into account, we compute *GW* corrected STM images and show that the contrast between the bare Si dimers and the C_2H_4 molecule is significantly improved with respect to DFT-LDA.

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Structural relaxation in excited states

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Abstract

The total energy surface (in particular, the resulting geometric equilibrium structure) of an excited electronic state is generally different from that of the ground state. The system will thus observe structural relaxation while being excited. Concomitantly, vibrational side bands will show up in the optical spectra. Such effects are discussed here for molecules and for the surface exciton at the Si(111)-(2x1) surface. The transition into the excited state is described by ab-initio techniques, including GW quasiparticle corrections and excitonic binding energies due to the electron-hole interaction.

Optical Properties of Semiconducting Conjugated Polymers: a First-Principles Study

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Abstract

The spatial extension and binding energy of excitons in semiconducting conjugated polymers is still the subject of intense debate. We address this problem through first-principles calculations (within DFT, plane-waves and ab-initio pseudopotentials), which allow to include electron-hole correlation effects in a fully 3D approach through the density-matrix formalism. We show results for the correlated optical spectrum and the exciton wavefunctions of single-chain and crystal poly(*para*)phenylene-vinylene (PPV).

Decay properties of the one-particle Green function in real space and imaginary time

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Abstract

The decay properties of the one-particle Green function in real space and imaginary time are systematically studied for solids. I present an analytic solution for the homogeneous electron gas at finite and at zero temperature as well as asymptotic formulas for real metals and insulators that allow an analytic treatment in electronic-structure calculations based on a space-time representation. The generic dependence of the decay constants on known system parameters is used to compare the scaling of reciprocal-space algorithms for the GW approximation and the space-time method.

Abstracts of Posters

Nonlinear magneto-optical Kerr effect in thin films from first principles

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Abstract

We present a first-principles calculation of the conductivity tensors relevant to study the linear and second-harmonic optical response from thin films. The calculations are done within the framework of the electric-dipole approximation and includes the Lindhard screening term. The formalism is presented. Numerical results are obtained using the WIEN95/97 FLAPW code with our own implementation of spin-orbit coupling and the optical response. The

films we consider consist of a monolayer of Fe and 1–7 monolayers of Cu. We show that the band structure and the density of states converge when we add more Cu layers to the structure. The nonlinear optical response, however, is much more difficult to converge than the electronic structure.

Electronic states and optical properties of heterostructures by pseudopotential calculations

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Abstract

The "linear combination of bulk bands" (LCBB) method [1] permits to calculate the single-particle electronic states of nanostructure systems, within an empirical pseudopotential framework. This method is particularly suitable for large scale superlattices, wires and dots, since it consists of writing the wave functions of the quantum states as linear combinations of Bloch eigenstates of the constituent bulk materials, over band indices n and wave vectors $\mathbf{k}$. The potential term in the Hamiltonian is built as a superposition of screened, spherical atomic pseudopotentials $v_\alpha(\mathbf{r})$, that are extracted from local density approximation calculations (LDA) on bulk systems and then adjusted empirically [2]. Unlike tight-binding or plane wave expansions, the LCBB expansion allows the intuitive pre-selection of physically important states to be included in the basis set, resulting in an easily manageable Hamiltonian matrix. Unlike $\mathbf{k}\cdot\mathbf{p}$ approach, off-Γ states $u_{n,\mathbf{k}\neq 0}$ are directly considered, eliminating the need for many $\mathbf{k}=0$ bulk states to describe $k \gg 0$ states. Moreover, the geometrical details of the structure are not lost and couplings are fully included. In this work we present the application of LCBB method to (001) superlattices (SL's). The band structure across all the tetragonal first Brillouin zone (BZ) is calculated for both $(\mathrm{GaAs})_m/(\mathrm{Alas})_m$ and $(\mathrm{GaAs})_m/(\mathrm{vacuum})_m$ SL's, for different values of m, and compared to bulk band structure folded in the tetragonal BZ. In $(\mathrm{GaAs})_m/(\mathrm{vacuum})_m$ SL's dangling bonds give rise to surface states which lie in the forbidden energy gap. The optical properties of these systems can be described, in first approximation, in terms of one-electron transitions produced by a perturbative electromagnetic Hamiltonian. The LCBB empirical pseudopotential approach allows calculations of optical spectra of heterostructures with a reasonably small computational time. Confinement and folding effects are well described [3]; on the other hand it isn't possible to neglect local field effects to account for optical anisotropies [4]

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Feynman histories and quantum measurements

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Abstract

Quantum measurement theory based on the von Neumann projection postulate [1] fails if the measured quantity relates to a finite duration rather than one instant of time. In this case a quantum system must be observed for a finite time and the measurement amplitude cannot, in general, be obtained by projecting its Schroedinger state on an eigenfunction of a hermitian operator. By defining a quantum measurement as destruction of coherence between certain components of Schroedinger wavefunction,we introduce a new approach which generalize von Neumann theory to finite time and continuous measurements. As examples of application of the new method, we analyze the quantum measurements of the traversal time [2] and the time average of a dynamical variable.

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An Excited State Density Functional Theory Study of the Rhodopsin Chromophore

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Abstract

Using a recently developed scheme for performing, within density functional theory, molecular dynamics and geometry optimisation for fairly large systems in the first excited singlet state, we have studied the structure and energy changes that the rhodopsin chromophore undergoes during the photoisomerisation from 11-cis to all-trans. We discuss the effects of relevant parts of the protein environment close to the chromophore on the isomerisation barrier and on the chromophore structure.

[C. Molteni et al., J. Am. Chem. Soc. 121, 12177 (1999)]

Cluster emission from crystal all-trans retinal

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Abstract

Electronic properties of retinal cromophores, and in particular of all-trans retinal, have been studied since long time in relation to the cis-trans photoisomerization of photoactive proteins(1). Much less is known about excited state dynamics in the crystal phase.

The fluorescence spectra of polycrystalline all-trans retinal (ATR) have been measured at 77 K as a function af exciting wavelength between 420 and 500 nm, i.e., below the energy of the lowest excited state of all trans retinal. By comparison with solution spectra at high concentration, emission from dimers and more associated species have been identified. On the same time, ab-initio calculations with the B3-LYP exchange-correlation functional and using the 6-31G* basis set have been performed on (ATR)n (n=2,3,4) species.

These calculations show that isolated clusters of all-trans retinal are stable in the ground state and suggest that these aggregates may be responsable of the observed fluorescence. It is hoped that theoretical ab-initio models may be developed to give a correct estimate of excited levels of clusters.

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Image Effects in Quantum Dots; a GW Approach

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Abstract

he significance of quantum dots for new physical insight on the nanoscale and future technical applications has long been recognised. As small quantum dots of nanometre size have moved into the realm of experimental feasibility, theory has yet to provide a comprehensive understanding of their underlying physics.

In contrast to a wide range of phenomena in quantum dots, image effects have not been intensively studied theoretically. Many-body effects in particular are aggravating accurate theoretical approaches. Based on a more qualitative and classical analysis of image effects [1], we pursue an approach by Saito *et al* [2] to apply the *GW* method to spherical jellium clusters. We developed a spherically symmetric formalism for the self-energy corrections, in which the dynamical screening of the Coulomb interaction includes these classical image effects, to testify the hypothesis proposed in [1]. An overall shift in the quasiparticle eigenvalues is observed, together with relative alterations in the energy spectrum, both of which are inherently absent in other methods such as density-functional theory. The work will subsequently be extended to fully realistic quantum dots.

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MIGS and Schottky barrier heights at non reactive GaN/noble-metal interfaces.

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Abstract

We present "ab-initio" FLAPW(a) calculations on N–terminated [001] ordered GaN/Ag and GaN/Au interfaces. Our results show that the density of gap states is appreciable only in the first semiconductor layer closer to the interface. The gap states decay length in the semiconductor side is about 3.8 a.u. and is independent on the deposited metal, therefore being to a good extent a bulk property of GaN. Our calculated values of the Schottky barrier heights for GaN/Ag and GaN/Au are respectevely 0.87 eV and 1.08 eV. Both these values are smaller than the GaN/Al(b) value 1.51 eV and this quite large spread of values excludes the possibility of a Fermi level pinning within the gap. This quite large variations of the Schottky barrier height as a function of the metal, in contrast with the behavior of GaAs/metal interfaces, are explained by the dependence of potential barrier on the structural arrangment of the first metal layer at the interface due to the low screening of GaN compared to GaAs.

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Optical spectra of complex surface structures

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Abstract

Optical spectroscopy of surfaces, in particular reflectance anisotropy spectroscopy (RAS) is a powerful and extremely versatile tool for *in situ* control of semiconductor processing with real-time feedback. The understanding and interpretation of the measured spectra, however, has been hampered by relatively slow theoretical progress.

We demonstrate that even for complex surface structures such as InP growth planes [1] and one-dimensional defects on Si surfaces [2] quantitative agreement between *first principles* calculations and experiment is possible, provided the calculations are numerically converged and self-energy corrections are included. Our calculations are done within DFT-LDA, using a massively parallel, real-space multigrid technique [3] to cope with the large supercells and many electronic states needed to calculate the surface dielectric function. Quasi-particle corrections are applied using a simplified GW scheme [4] or a scissors operator approach. We identify two distinct sources for the optical anisotropy: (i) highly structure-dependent features are caused by transitions involving electronic surface states, and (ii) derivative-like oscillations or peaks at the bulk critical point energies arise from transitions between surface-modified bulk wave functions. Two mechanisms cause anisotropy signals from layers beneath

the surface: the influence of the anisotropic surface potential on the bulk wave functions as well as minor contributions from atomic relaxations caused by surface-induced stress.

[1] WG Schmidt *et al.* Phys. Rev. B **61**, R16335 (2000).

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6.2.3 Report on the Brighton Conference

Report on the Conference on Extended Defects in Semiconductors 2000 University of Sussex at Brighton, 18th - 22nd July

The conference was opened by Schroeter (Goettingen) who succinctly summarised the main developments in our understanding of dislocations over the last 30 years. Of crucial importance had been the application of experimental techniques like DLTS, PL and EPR, as well as theoretical modelling, to extended defects. Nevertheless, fundamental questions remain with regard to understanding their generation, mobilities, electronic and optical properties, and these have become even more relevant with the emergence of new technologically important materials like GaN. Working nitride LEDs contain dislocations with densities of order 10^{10} cm^{-2} whose presence in other III-Vs like GaAlAs would be fatal to optical devices.

The first sessions of the conference by Nunes (Rutgers), Csanyi (MIT) and Justo (Sao Paulo) described results from large scale calculations of the structure and line energies of dislocations, kinks and soliton defects. These generated active discussion prompted by questions from experimental groups. The next talks by Jacques (Nancy), Rabier (Poitiers) and Yonenaga (Sendai) explained how TEM, X-ray and etch pit methods were able to demonstrate that dislocations in Si multiplied by cross slip, were affected by high pressures, and could be pinned by boron clus- ters. Leipner (Martin Luther) then reported on calculations of large vacancy clusters (10 and 14 atoms) in plastically deformed Si and GaAs which are observed in positron annihilation experiments.

The second day began with an excellent talk by Maeda (Tokyo) on hydrogen and recombination enhanced dislocation motion including radiation enhanced vibrational movement. These were illustrated in Si, GaN and ZnO. The origin of the effects was not always clear and generated a considerable discussion. Then five talks on the electronic and optical properties of plastically deformed Si probed by EBIC and PL, and analysed theoretically. These contributions generated much heat and controversy. Are the PL bands due to oxygen (Pizzini, INFM) or interstitial point defects attached to the line (Blumenau, Exeter), or are they just due to isolated defects (Higgs, BioRad)? Does the explanation of their temperature dependence really require a band of states associated with a stacking fault (Weber, Dresden)? The conference clearly highlighted these crucial questions and the many questions raised will doubtless spur further investigations.

Wilshaw (Oxford) described how dislocations trap oxygen implying an enhanced diffusion possibly due to dimers while Markevich (Manchester) found hydrogen to lead to enhancements in oxygen diffusion at high temperatures. Clearly, many of these new experimental results will tax will the theorists present!

Defects in GaN were a major concern. Several talks dealt with irradiation defects (Cavallini,

Bologna), defects introduced by etching (Weyher, Nijmegen), indentation (Albrecht, Erlangen; Pirouz, Case Western), and by growth (Ponce, Xerox; Ruterana, ESCTM-CRISMAT). There is much work for theoreticians in this area but their task is made the harder by contradictory exper mental results. For example, are glide dislocations dissociated? Doubtless, more careful experiments will be reported in future.

Cherns (Bristol) described the harmful effects of large piezo- electric fields in GaInN quantum wells arising from mismatch while Northrup (Xerox) demonstrated the power of computational modelling in anticipating the structure and properties of inversion boundaries in the nitrides. Mooney (IBM) emphasised the role of strained Si as promoting electron mobility but the deleterious effect of misfit dislocations. Batson (IBM) demonstrated the power of new techniques like EELS to give detailed structural properties of dislocations in Si while Brown (Nottingham) re- ported on the first oxygen extended defect found in GaN.

Stach (Berkeley) showed a video of worm holes in GaN caused by nitrogen desorption while Chisholm (Cambridge) reported calculations showing that stacking faults were more stable in Si doped material.

Dislocations and atomic migration in fullerenes and graphite (Ewels, Sussex) demonstrated that fundamental concepts such as interstitial assisted diffusion have applications outside Si while a riveting talk by Brown (Cambridge) on platelets in diamond further demonstrated the power of EELS measurements nicely explained by the modelling studies reported by Goss (Exeter). Finally, Heggie (Sussex) presented results of first principles modelling of the effect of H plasmas on dislocations in silicon and diamond.

The excellent lectures given by all and the unresolved issues, made the conference a great success and convinced everyone of the importance of a follow up meeting in two years time.

R. Jones (Exeter) and M.I. Heggie (Sussex)

Abstracts

Extended Defects in Semiconductors 2000

University of Sussex at Brighton
July 18th - July 22nd

Tuesday 18th July

Session 1: Mike Duesbery Memorial session. Structure and motion of dislocations in silicon

Chair: Amand George

The double-period structure of the 90° partial dislocation in homopolar semiconductors

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Department of Physics and Astronomy - Rutgers University
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Abstract

The 90° partial dislocation in silicon has been known to undergo a symmetry-breaking core reconstruction, with atoms bonding in pairs along the zigzag chain that forms across the dislocation line, leading to a relatively simple geometry which preserves the underlying-lattice periodicity in the dislocation direction. This reconstruction is apparently the natural way of restoring the fourfold coordination of the atoms in the core, and since the late 70's has been the basis of virtually all theoretical work on this defect. Recently, this picture has been questioned by our ab initio calculations [J. Bennetto, R. W. Nunes, and D. Vanderbilt, Phys. Rev. Lett. 79, 245 (1997)] which revealed that a period-doubling reconstruction, obtained by inserting kink-antikink pairs along the core of the traditionally accepted structure, is actually lower in energy. Our original work, which addressed the case of silicon, was later extended to include germanium and diamond [R. W. Nunes, J. Bennetto, and D. Vanderbilt, Phys. Rev. B. 58, 12563 (1998)], leading to the observation that the energy gain associated with the new reconstruction follows the same trends as the gaps and the stiffness in these materials. This talk contains a review of these theoretical developments on the double-period structure of the 90° partial. Preliminary results on a comparative study of the structure and diffusion barriers of vacancies on both core structures will also be reported.

New physics of the 30° partial dislocation in silicon revealed through ab initio calculation

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Abstract

Based on ab initio calculation, we propose a new structure for the fundamental excitation of the reconstructed 30°partial dislocation in silicon. This soliton has a rare structure involving a five-fold coordinated atom near the dislocation core. The unique electronic structure of this defect is consistent with the electron-spin-resonance signature of the hitherto enigmatic, thermally stable R center of plastically deformed silicon. Furthermore, the free energy of these defects, calculated with a novel thermal sampling technique applied for the first time to ab initio calculations, is sufficiently low to explain the predominantly high density of R centers in annealed, plastically deformed silicon. This identification suggests the possibility

of an experimental determination of the density of solitons, a key defect in understanding the plastic flow of the material.

Dislocation Core Effects on Type IV and III-V Semiconductors

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Abstract

Dislocations in semiconducting materials are known to affect both the electronic and mechanical properties of the materials. In silicon, dislocation mobility is low at normal operating conditions. On the other hand, under equivalent conditions, dislocation mobility is considerably higher in III-V and II-VI compounds. Considering that all these materials have the same crystalline structure and therefore the same type of dislocation activity, it is relevant to identify the origin of such large scatter of dislocation velocities.

Here we have investigated the energetics involved in core reconstruction of partial dislocations in several zinc-blende semiconductors and correlated those energies to the experimental activation energies for dislocation motion. Core reconstruction of {111} 30°glide partial dislocations in polar and non-polar semiconductors was examined using ab initio total energy calculations. The ab initio calculations were performed within the density functional theory and the local density approximation. Norm-conserving pseudopotentials were used to model the ionic potential and the valence electron wavefunctions were expanded in a plane-wave basis set. Theoretical results for the core reconstruction energy of 30°partial dislocations are for the first time directly correlated to the experimental activation energies for dislocation velocity of 60°dislocations in zinc-blende materials. Additionally we have investigated the electronic properties of unreconstructed and reconstructed core structures, and a new model for the electronic band structure associated with the dislocation core is proposed.

Session 2: Structure and motion, including impurity and point defect interactions

Chair: Bob Jones

Dislocation multiplication at the onset of plasticity in Si observed by in situ Synchrotron X-Ray topography

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Abstract

Dislocation creation and multiplication were investigated in silicon in creep conditions on initially dislocation free tensile samples (ca.15 x 4 x 0.7 mm), with resolved shear stress in primary slip systems in the range 10-20 MPa, at temperatures from 980 K to 1100 K. The very first dislocations were created by Vickers indentations. Using the high intensity X-rays of the ID 19 beamline of the ESRF, series of "snapshots" were taken as dislocation loops expanded, till the overall density approached the limit value that can be resolved by X-ray topography. Burgers vector and stereographic analysis was performed post-mortem by Lang topography.

Observations revealed:

i) creation of the first dislocations (in several slip systems) only at surface defects.

ii) several cases of cross-slip over large distances, initiated either at a free surface or in the bulk..

iii) formation of different source configurations, either by double cross slip, or by interaction of dislocations of different slip systems. The most efficient sources had a stable pole formed by reacting dislocations of different slip systems.

iv) a general trend for trails of dislocations emanating from one source to become less planar and more dense, with rectilinear dislocation segments turning to wavy lines.

Dislocation Activities in Heavily Impurity Doped Si

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Abstract

Interaction between dislocations and impurities in semiconductors has two interesting aspects.One is the effect of dislocations on the spatial distribution of impurities in a crystal. The other is the effect of impurities on dynamic activities of dislocations. O and N are known as impurities with strong effects of dislocation immobilisation.Contrarily, far less is known of the effects on dynamic activities of dislocations by electrical, especially acceptor, impurities. Recently, Si crystals highly doped with electrically active impurities are used as a substrate material for the epitaxial growth of the clean Si with no grown-in defects. In addition, recent large diameter Si wafers are under a condition of easy dislocation generation by the self weight. Thus, it becomes very important to clarify the dislocation activities in such highly impurity doped materials from both practical and fundamental viewpoints.

Dynamic behaviour of dislocations in Si crystals doped with B, P, As, etc. in various concentrations up to 1.5 x 1020 cm^{-3} has been investigated as a function of stress and temperature in comparison with that of dislocations in undoped and O-doped Si. Specimens free from dislocations were prepared from Si grown by the Czochralski (CZ) and float-zone (FZ) techniques. Dislocation generation and motion were directly characterised by means of the etch pit method. In impurity doped Si there is a critical stress for dislocation generation from a scratch drawn as a preferential generation site: For example, the magnitude of the critical stress is as high as approximately 15 MPa in B-doped CZ-Si in a concentration of 8.8 x 1019 cm^{-3}, while that is 0 and 8 MPa in undoped FZ- and CZ-Si, respectively. Donor impurities show such a suppression effect for dislocation generation in a concentration lower than that of B impurity by an order of magnitude. The critical stress for dislocation generation increases with increasing impurity concentration. The critical stress was determined as a function of impurity concentration and temperature. At stress higher than the critical stress, the dislocation velocity in the B-doped Si in the various concentrations is almost comparable to that in undoped FZ- and CZ-Si. On the other hand, donor impurities enhance dislocation velocities. Such dislocation behaviour in impurity-doped Si is interpreted in terms of dislocation locking due to impurity clusters and/or impurity-defect complexes. Impurity effects on dislocation activities in Si will be summarised.

Vacancy clusters in plastically deformed semiconductors

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Abstract

Experimental investigations of plastically deformed elemental and III-V semiconductors prove that a high number of vacancies and vacancy clusters is formed. The formation of point defects by different types of moving jogged dislocations is analysed. Vacancies formed behind the jog are not stable as a simple chain of vacancies. Instead, they are transformed to stable three-dimensional agglomerates. No diffusion step is required for this transformation. It occurs close to the dislocation, and the association of the vacancy clusters with the dislocation may be likely. The stability of various vacancy clusters has been investigated by density-functional calculations [1]. The positron lifetime in such clusters was calculated and compared to experimental results. The association of open-volume defects with the dislocation can be derived from positron lifetime measurements. The analysis in a positron trapping model characterizes the dislocation as a combined defect. The undisturbed dislocation line is a precursor trap for the positron capture in a deep trap related to the vacancies bound to the dislocation.

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Wednesday 19th July
Session 3: Structure and motion of dislocations

Chair: Pirouz Pirouz

Dislocation motion under the influence of electronic perturbations

Koji Maeda, K. Suzuki, Y. Yamashita and Y. Mera

Abstract

In spite of the innocuousness of dislocations in GaN-based optoelectronic devices, the dislocation glide motion in GaN is actually enhanced by electronic excitation. Comparison is made with other wide-gap semiconductors such as SiC and ZnS, together with ZnO for which our recent in-situ TEM observations showed that the dislocation glide in this solid is also enhanced by electron beam irradiation. Also the origin of the peculiar low-frequency vibrations of dislocations, found in ZnO too, will be discussed.

T.E.M. in situ investigation of dislocation mobility in semiconductors

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Abstract

T.E.M. in situ straining experiments provide a unique way to investigate in real time the behaviour of individual dislocations under applied stress. The results obtained on a variety of semiconductors are presented. Numerous dislocation sources are observed which makes it possible to measure the dislocation velocity as a function of different physical parameters (local shear stress, temperature, dislocation character, length of the moving dislocation ...). The experimental results are consistent with a dislocation glide governed by the Peierls mechanism, even in II-VI compounds which have a significant ionic character.

In III-V and II-VI compounds, a linear dependence of the dislocation velocity with the length of the moving segment is noticed. Analyzed in the frame of the kink diffusion model (Hirth and Lothe theory) this result indicates that dislocations move in the kink-collisionless regime. Kink formation (Fk) and migration (Wm) energies can be estimated from these experiments. Compared to elemental semiconductors, the ratio Wm/Fk is rather low, which suggests that dislocation cores are not reconstructed in these compounds.

In a variety of semiconductors the dislocation behaviour is sensitive to photonic or electronic excitations. T.E.M. in situ straining experiments have been conducted in ZnS and ZnSe with attention to the effect of electron beam on the dislocation motion. A strong increase of dislocation mobility with increasing electron beam intensity is observed (radiation enhanced dislocation glide). It is attributed to a lowering of the lattice friction, due to non-radiative recombinations of electronic carriers at dislocation sites.

The limitations of the technique, as well as the possible artefacts, will be discussed.

Deformation of Semiconductors at Low Temperatures

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Abstract

Plastic deformation of four III-V compounds, GaP, GaAs, InP and InSb, have recently been performed at low temperatures (77-500K) under confining pressure[1-4]. Their critical resolved shear stress tc reveals similar temperature dependence: strong temperature dependence at low temperatures (regime I), weak and plateau-like dependence at intermediate temperatures around 300K (regime II) and still stronger dependence at high temperatures (regime III). This results in a clear hump at about 300K. Throughout the three regimes I-III, slip lines are always wavy, indicating frequent cross-slips of screw dislocations. Furthermore, even around 700K and under ambient pressure (regime IV) GaAs and InP exhibit wavy slip traces, contrary to Si [5].

These observations seem to contradict the assumption that plasticity of semiconductors is governed by kink processes of dislocations dissociated in the glide set planes, and suggest that undissociated screw dislocations are dominantly responsible for the plastic straining.

Computer simulation shows that for an undissociated screw dislocation the lowest energy position is not the center of a unit $< -101 >$ hexagon, but on the longer edges of the hexagon [6]. This allows two paths for kink pair formation on the screw dislocation in the {111} shuffle plane: a planar path at high stress and a zig-zag path at low stress. The transition between the planar path at low temperature (regime I) and the zig-zag path at high temperature (regime III) describes the plateau and hump in the tc -T curves [4].

The difference between elemental semiconductors (Si and Ge) and III-V compounds will be discussed.

References:

[1] T.Suzuki, T.Nishisako, T.Taru and T.Yasutomi: Phil. Mag. Lett., 77, 172 (1998).

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Session 4: Characterisation I

Chair: Sergio Pizzini

Quantitative model for EBIC-contrast and PL of dislocations decorated by metallic impurities

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Abstract

Existing experimental data give much evidence that the recombination rate of minority charge carriers at dislocations in Si depends strongly on dislocation decoration by transition metal impurities. Here, we present a model, which allows a description of recombination of minority carriers on decorated dislocations. This model assumes dislocation energy bands, induced by a strain field, and deep electronic levels, caused by impurity atoms in the vicinity of the dislocation core (or by core defects). The model is based on the idea that these deep levels can capture charge carriers from the dislocation energy bands. As a consequence the recombination of carriers captured at dislocation bands can be drastically enhanced by the presence of even small concentrations of impurity atoms at dislocation core. The model allows not only to explain experimentally observed dependencies of recombination rate on temperature and excitation level, but also to estimate the concentration of deep level impurity at dislocations.

Combined with EBIC investigations of sample with well controlled contamination and extended to higher temperatures, the model opens a quantitative access to segregation and electronic structure of metallic impurities at dislocations.

Room temperature luminescence from dislocations in silicon

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Abstract

A review is presented on the temperature dependence of the D-band luminescence in Si. In detail, we will discuss the temperature induced changes of the line positions, the linewidth and the excitation dependence. A strong influence of the luminescence intensity is detected on sample preparation and defect contamination. Room-temperature luminescence from the D-bands can be generated in floating zone samples with reduced contamination of transition metals and oxygen. The electroluminescence from pn-junctions which contain dislocations in the space charge region is similar to the photoluminescence in these samples. The intensities of forward biased n+p-diodes will be compared with the corresponding photoluminescence intensities and different recombination processes will be discussed

Photoluminescence characterization of defects in Si and SiGe structures: The influence of transition metal impurities

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Abstract

The optical and electrical activity of defects in semiconductors has been studied in detail by numerous methods. Low temperature Photoluminescence (PL) spectroscopy on dislocations in Si has long established that certain luminescence features can be attributed to the presence of dislocations. The main dislocation features are the D1-D4 bands (D-bands). Although they have been the subject of many detailed evaluations there is still speculation over their exact origin. There is clear evidence that the transition metal impurities may play a key role in the dislocation-related luminescence. Combined CL and EBIC studies have produced a clearer picture in understanding the role of impurities on the activity of dislocations in Si and SiGe. In light of the renewed interest in understanding the optical and electrical activity of dislocations the PL results will be reviewed and summarised.

From a technological point of view it is more important to detect the presence of dislocations irrespective of their electrical activity in Si., because subsequent device processing of Si wafers containing dislocations will almost certainly lead to poor device performance and low reliability. A new room temperature PL method has been developed to detect defects in the near surface region of Si wafers and SiGe structures. Wafer maps (up to 300 mm) can be readily acquired and areas of interest can be scanned at high resolution (1 μm). The excitation laser beam is modulated to confine the photogenerated carriers; defects are detected due to the reduction of the localised recombination lifetime. Examples will be shown of PL maps revealing dislocations in Si, and misfit dislocations in SiGe and the influence of transition metal contamination.

The D1 to D4 optical bands related to dislocations in Si

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Abstract

The properties of multi-vacancy and multi-interstitial defects that possess luminescent bands around one eV are reviewed. Prominent among these are the hexavacancy and tri- and tetra- self-interstitial defects. It is suggested that the formation of these defects on dislocation cores could lead to the D1 to D4 photoluminescent bands linked to dislocations in Si and SiGe.

Session 5: Characterisation II

Chair: Vitaly Kveder

Spectroscopic study of the PL emission in the 0.7-0.8 eV range from oxygen precipitates, thermal donors and dislocations in silicon

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Abstract

In a previous work we have studied the photoluminescence of dislocated and oxygen segregated samples of semiconductor silicon [1] and we were able to show that a PL band at 0.85 eV at 16 K is correlated with oxygen segregation at dislocations. We were also able to show that this result fits with a variety of other misinterpreted literature reports and that PL emission from clean and oxygen segregated dislocations has a different temperature dependence, which does allow to distinguish in a sufficiently clear way the two different light emission processes.

This last result was possible also thanks to the availability of a matrix of samples in which the oxygen was segregated with carefully selected nucleation and precipitation stages, under the very clean conditions of a VLSI process.

In this presentation we intend to review our previous work as well as to present and discuss some new results dealing with the photoluminescence of thermal donors, in the frame of a very careful analysis of previous literature reports.

We will show that the emission at 0.778 eV, which was associated by Steinman and Grimmeis [2] to a radiative transition between a dislocation acceptor and a thermal donor level, is present also in undislocated but thermally treated samples and that it follows a very puzzling dependence on the donors concentration.

We intend to show that the PL emissions in the 0.7-0.8 eV range is correlated with the oxygen segregation in form of oxygen clusters at dislocations or in the bulk and we intend to propose a new realistic model for the light emission processes in this energy range.

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The interaction of oxygen with dislocations in Czochralski Si

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Abstract

Locking of dislocations by oxygen atoms in Czochralski-silicon has been investigated both experimentally and theoretically. Experiments were performed at annealing temperatures between 350°C and 850°C for different annealing times and different oxygen concentrations. These showed five distinct regimes for the unlocking stress as a function of annealing time. First the unlocking stress increases almost linearly with time and then saturates. The saturation stress, time needed to reach the saturation and duration of saturation depend on annealing conditions and oxygen content. Following the saturation a rapid increase and a second saturation of the unlocking stress with increasing annealing time were observed. Finally after long anneals the locking effect is much reduced. From the temperature dependence of the first saturation stress the interaction energy between an oxygen atom and a dislocation has been deduced and it is shown that the change of entropy when an oxygen atom is trapped at a dislocation is significant. The transport of oxygen to dislocations has also been investigated by solving the diffusion equation numerically. For these calculations both trapping and emission of oxygen atoms from the dislocation core have been considered and values obtained for the diffusivity of O in the temperature range 350°C to 850°C.

Hydrogen-plasma-enhanced oxygen precipitation in silicon

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Abstract

High temperature (650 - 1100 ° C) treatments of Czochralski-grown silicon crystals are known to result in the loss of oxygen atoms from solid solution and the generation of extended defects in the form of different oxygen-related precipitates. These defects are widely used in microelectronic technology for gettering various undesirable metallic impurities.

It was shown in earlier work that the presence of hydrogen in Cz-Si crystals leads to enhanced oxygen diffusion and thermal double donor formation in the temperature range of 300 - 450 ° C [1]. In the present study, infrared absorption measurements (FTIR) have shown that the loss of oxygen and formation of oxygen precipitates is strongly enhanced in bulk Cz-Si samples which have been heat-treated in a hydrogen plasma at a temperature in the range 500 - 700 ° C. Possible mechanisms of the enhanced oxygen precipitation will be discussed and some applications of the observed effect will be considered.

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Secondary extended defects in the slip plane of moving dislocations in Si

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Abstract

In the previous investigations a new kind of extended defects, generated by moving dislocation was revealed in Si and SiGe [1]. It was found that the elements of defect morphology and etching behaviour completely differ from those of the traditional defects. A motivation for further experiments was to understand completely defect morphology and the nature of the phenomenon.

In this paper some key experimental results are presented, which could essentially change our ideas about properties of moving dislocations in diamond lattice [2,3]. It is shown that new secondary defects are revealed in the dislocation slip plane as dense rows of ridges with extraordinary (hundreds of microns) length and are generated namely by moving dislocation. An analysis shows, that likely only 60°glide dislocation is active. Very likely, the defects are similar to well known rod-like defects. The results are discussed in terms of an atomic level dislocation core reconstruction as a source of a very high density of intrinsic point defects. In that case the experimental data on SiGe alloys are of particular interest.

An intriguing result was obtained after analysis of electrical activity of the defects. Contact-less detection method of surface electron induced voltage in SEM was used. Noticeable recombination activity of the defects was discovered. The fact is quite unexpected and possibly may be considered as a "new page" in understanding of dislocation and point defect properties in covalent lattice. It is supposed that the defect generation is a specific lattice phenomenon for diamond-like materials and, possibly, for III-V and II-VI compounds. A possible correlation between existence of the defects and low temperature plasticity and brittle-ductile transition in Si as well as some electronic properties of dislocations are considered.

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Session 6 : Characterisation continued, including III-V and II-VI

Chair: Peter Wilshaw

Deep-level defects at lattice mismatched interfaces in GaAs-based heterojunctions

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Abstract

Electrical properties of lattice-mismatch-induced defects in GaAs-based heterojunctions have been studied by means of electron-beam-induced current (EBIC) in a scanning electron microscope and deep-level transient spectroscopy (DLTS).

Two types of heterostructures, p^+-n GaAs/GaAsSb junctions (0 to 3% Sb content) grown by liquid phase epitaxy and n^+-p GaAs/InGaAs junctions, (3% In content) grown by molecular beam epitaxy, were investigated. A difference in lattice constant between GaAs and the ternary compound (about 0.2% at 3% of Sb or In content) resulted in generation of misfit dislocations at the interface to relieve some of the strain in the epitaxial layer. A two-dimensional array of and misfit dislocations gliding along two orthogonal $< 110 >$ directions at the (001) interface has been visualized by means of the EBIC technique in both types of heterostructures.

DLTS measurements, carried out with p-n junctions formed at the interfaces, revealed one electron trap and two hole traps induced by the lattice mismatch. The electron trap, at about E_c - 0.65 eV, has been attributed to electron states associated with misfit dislocations. By comparing the concentration of this trap, revealed by DLTS, with EBIC results of diffusion length, obtained in heterojunctions with different lattice mismatch, it is inferred that the minority-carrier lifetime is controlled by dislocations in the epilayer region close to the interface.

Deep levels and irradiation effects in n-GaN

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Abstract

GaN-based wide-band-gap III-V compounds currently attract a wide interest because of the extensive number of applications they can cover as light emitting diodes, detectors and lasers. In spite of the large effort to assess their characteristics, there are still many open questions on their physical properties and on the defects which control them. The best way for studying defects is to create them in a controlled manner by irradiation.

This contribution deals with the characterization of the defects existing in HVPE-grown undoped n-GaN and their changes induced by proton irradiation. The energy position in the gap of deep levels has been investigated by spectral photocurrent measurements, DLTS and steady-state photo-capacitance analyses. It has been found that new defects appear after irradiation and that the features of some of the pre-existing defects change. Results of persistent photoconductivity before and after irradiation are also presented and related to the electrically active defects.

Defects in GaN epitaxial layers and single crystals: etching and TEM studies

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Abstract

GaN single crystals and particularly hetero-epitaxial layers contain diversity of structural and chemical defects. Transmission Electron Microscopy and high resolution X-ray diffraction were up to now most frequently used to determine structural quality of epitaxial layers and single crystals, see e.g. [1-3]. Defect-selective etching, which is known as quick and inexpensive method of structural data acquisition in elemental and compound semiconductors, remains far behind the use of these methods due to the known high chemical resistance of nitrides as well as due to the polarity-related strong anisotropy of properties.

In this paper the use of different chemical defect-selective etching methods, recently developed for study of defects in GaN, will be summarized. Etching in: (i) hot phosphoric and sulphuric acids (denoted HH etch), (ii) molten KOH-NaOH bases (denoted E-etch), (iii) photoelectrochemical (PEC etching) in aqueous KOH solutions and (iv) electrochemical etching in KOH solutions will be critically compared. The ability of revealing by these methods of the variety of defects, such as inversion domains, nano-pipes, dislocations, stacking faults and growth striations will be demonstrated. The evidence will be presented that the size of etch pits formed on grown-in dislocations in GaN single crystals is remarkably higher than the size of pits formed on dislocations introduced by indentation at low temperature. This effect has been well recognized in other III-Vs, e.g. GaAs, and attributed to the different degree of decoration of individual dislocations.

Since etching technique belongs to the indirect methods used for structural characterization, examples of calibration of etch features by TEM will be shown.

[1] P.D. Brown, J. Crystal Growth 210 (2000) 143.
[2] P. Prystawko et al. J. Crystal Growth 198/199 (1999) 1061.
[3] M. Leszczynski et al., Appl. Phys. Lett. 75 (1999) 1276.

Optical characterization of isolated Se(g)-type misfit dislocations and their influence on strain relief in thin ZnSe films

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Abstract

We have been able to obtain microscopic information on dislocations in ZnSe layers grown on (001)GaAs substrates by molecular beam epitaxy using micro cathodo- and photoluminescence. Whereas high quality pseudomorphic films are dislocation free, above the critical thickness 60°dislocations are incorporated. The Se(g) type misfit dislocations are found to nucleate first. They form bunches of defect lines aligned collinearly to the in-plane direction. This asymmetric defect configuration results in an anisotropic stress relief and causes unexpected changes of the spectral and polarization characteristics of the layer luminescence. The so called Y luminescence line at 2.6eV is shown to be directly correlated with a dislocation bound exciton state. Our experiments yield that the strain field of a 60°dislocation segment can be mapped by studying the lateral dependence of the luminescence. The individual Se(g) misfit segments are evidenced as the only local emission centers of the Y-luminescence which is strongly polarized in defect line direction and exhibits a pronounced spectrum fine structure. The latter is recognized to be an inhomogeneous property related to the particular dislocation structure, as determined by the dissociation of perfect dislocation segments into pairs of Shockley-partials bordering a stacking fault ribbon.

The observed local dependence of free and bound exciton emission, in particular, the spectral shift, splitting and polarization of the luminescence peaks is interpreted in terms of spin Hamiltonians incorporating the influence of local strain, internal electric fields and electron-hole exchange interaction on the electronic structure of excitonic states. The dislocation-induced luminescence is ascribed to 1D excitonic states at the line defect. The origin of a two sub-components feature appearing in the Y-luminescence spectrum when a single dislocation is monitored, is studied by applying high magnetic fields. By investigating the anisotropy of the Zeemann-splitting the electron-hole exchange interaction is found to play an important role for the dislocation-bound excitons.

The local strain field as displayed by spectral and polarization characteristics, extracted for the Se(g) misfit segments as well as layer matrix is utilized to discuss the lattice relaxation just above the critical layer thickness.

Thursday 20th July
Session 7: Extended Defects in IV-IV compounds

Chair: Ichiro Yonenaga

Plastic behaviour of SiC single crystals

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Abstract

Plasticity of elemental and III-V compound semiconducting materials has been extensively studied in a wide range of stress and temperature. However, data on the yield stress and other plastic properties of IV-IV compounds, e.g. different SiC polytypes, is lacking mainly because until recently it was not possible to grow single crystals of these materials in large dimensions. In the last few years, reasonably high quality bulk single crystals of 4H-SiC and 6H-SiC are being grown by the modified Lely technique and wafers cut from these bulk ingots are now commercially available. Recently, compression experiments on the new high-quality 6H and 4H-SiC crystals at different strain rates have been performed in order to measure the yield stress, ty, as a function of temperature, T. A break in the ln(ty) versus 1/T plot at a critical transition temperature Tc is observed which corresponds to a change in the deformation mechanism characterized by TEM. Indeed, observations show that at $T > T_c$, the microstructure consists of pairs of leading/trailing partials associated with the dissociation of perfect dislocations, whereas at $T < T_c$ only single leading partial dislocations, each of them dragging a stacking fault, can be observed. The critical transition temperature T_c appears to be close to the brittle to ductile transition (BDT) temperature. In this talk, results of recent experiments are presented and the relation of the transition in deformation mode to the transition in fracture mode (brittle to ductile) is discussed.

Microstructure of Strain-Relaxed SiGe/Si Heterostructures

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Abstract

Strain-relaxed Si1-xGex alloy films on (001) Si substrates serve as buffer layers for field-effect transistors having strained Si or Si1-yGey ($y > x$) carrier channels. At low mismatch strain ($< 2\%$), SiGe/Si(001) heterostructures relax by the introduction of 60o misfit dislocations. The presence of dislocations results in the broadening of the x-ray rocking curve peak from the SiGe layer. Triple-axis x-ray diffraction measurements indicate that this is primarily "mosaic broadening" resulting from local tilting of the lattice planes, caused by the misfit segments of the 60o dislocations. Recently we have used spatially resolved x-ray beams at the NSLS (X20) and at the APS (2ID) to investigate the microstructure of relaxed SiGe films. Samples that relaxed by different dislocation nucleation mechanisms and therefore are expected to have different microstructure were investigated. These two types of samples were: step-graded structures consisting of a series of thin layers, each with increasing Ge mole fraction, followed by a thick (1-4 μm) uniform composition layer and samples having only a uniform composition Si1-xGex ($x > 0.2$) layer.

Measurements taken at the NSLS (X20), using a divergent beam focussed by a tapered capillary, show that the intensity of the diffracted beam varies as the sample was stepped under the incident beam. Rocking curves and detector scans taken at different positions on the sample show local regions that have a similar lattice parameter but are tilted at various angles with respect to the substrate [1,2]. These regions form during the initial stages of relaxation and, as the dislocation density increases, the tilt angles also increase. The size of the local tilted regions is 10-20 μm. Data taken with a parallel beam at the APS (2ID) indicate that these relatively large regions consist of smaller tilted regions, on the order of 1 μm, that have a relatively narrow distribution of tilt angles. Local tilted regions were also observed in uniform composition SiGe layers at the APS (2ID), using the first order beam from a zone plate that is an order of magnitude smaller in size. The tilted regions in these films are on the order of 1 μm in size but are randomly distributed.

* Partially supported by DEO contracts DE-AC02- 76CH00016 and W-31-109-Eng-38.

[1] P.M. Mooney, J.L. Jordan-Sweet, I.C. Noyan, S.K. Kaldor and P.-C. Wang, Appl. Phys. Lett. 74, 726 (1999).

[2] P.M. Mooney, J.L. Jordan-Sweet, I.C. Noyan, S.K. Kaldor and P.-C. Wang, Physica B 273-274, 608 (1999).

Session 8: Extended defects in IV-IV compounds continued

Chair: Wolfgang Schroeter

Spatially Resolved EELS Study of a Misfit Dislocation in GeSi

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Abstract

Silicon $L_{2,3}$ EELS spectra have been obtained from several positions within the structure of a dissociated 60° misfit dislocation at the substrate interface of a strained $Ge_{30}Si_{70}/Si/Ge_{30}Si_{70}$ quantum well. These spectra have been obtained using 0.2eV energy resolution and a 0.2nm probe in the VG Microscopes HB501 STEM operated at 120KV. Annular Dark Field imaging at the 0.2nm level allows correlation of the spectra with particular atomic level structure near the dislocation. Detailed interpretation of the spectra, based on prior work in strained and relaxed SiGe alloys, reveals the symmetry- and site-projected bandstructure of the solid. In this case, the dislocation dissociates into the well-known 30°-ISF-90° structure. ADF imaging reveals the 30° partial to be the glide cut structure with one atom column at its core. The ISF is 10 double atom units long, terminating in the 90° partial. Imaging at the 90° core does not conclusively reveal its structure, but does strongly suggest that a simple single period reconstruction would not be adequate to understand the structure. EELS spectra from the GeSi reveal structure attributed to Δ_1, L_1 and L_3 in the Brillouin Zone. Near the dissociated dislocation, several effects are observed. Within 1.5 nm, but not at central points of symmetry, contributions from both Δ_1 and L_1 are shifted and split by local

strain. These are consistent with resulting CB shifts of ± 200meV in the regions of tension and compression on either side of the dislocation. On the ISF, the L_1 band is split into two contributions, a consequence of the broken crystal symmetry. Δ_1, on the other hand is not affected. At the partial dislocations, in-gap states near the CB edge are prominent. At the 30° partial, the L_1 band splits in a manner very similar to that seen at the ISF. It can be argued that this is a consequence of the pairing reconstruction that is expected at that core. On the other hand, this splitting is not observed at the 90° partial, in spite of the fact that all currently suggested core models include local structure that might be expected to produce ISF-like electronic behavior. An extended, kink-based core model, derived from the recently proposed Double Period reconstruction for the 90° partial dislocation, is suggested to understand this finding. [1, 2]

[1] P.E. Batson, Phys. Rev. Lett. 83, 4409 (1999).

[2] P.E. Batson, Phys. Rev. B 61, 16633 (2000).

Friday 21st July
Session 9: Extended defects in III-V compounds

Chair: Eicke Weber

Film defects and growth dynamics in gallium nitride epitaxy

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Abstract

The outstanding performance of the nitrides as bright emitters for blue and green light is associated with a number of unexpected physical observations. The substrate of choice for devices, sapphire, does not reflect optimization in lattice mismatch nor of thermal expansion difference, traditionally believed necessary for high optoelectronic quality epilayers. High performance films exhibit the absence in thermal stresses that should be pronounced due to the bulk properties of sapphire and GaN (which differ by almost 50% in the thermal expansion characteristics). And large dislocation densities (of the order of 1010 cm^{-2}) appear to be necessary in order to achieve superior electronic performance, contrary to the tendencies in other semiconductor systems where dislocations are known to be highly detrimental to performance. In this talk, the rich microstructure of GaN films on sapphire will be explored, and its relationship with the surprisingly superior optical and electronic behavior will be discussed

The multiple atomic configuration and formation mechanisms of the extended defects in Ga based wurtzite nitrides

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Abstract

Extensive experimental investigation has been carried out by high resolution electron microscopy on most of the known extended defects (threading dislocations, inversion domain boundaries and stacking faults).

The threading dislocations have their lines which are mainly parallel to the growth axis and more than 90% are of a type. It was then possible to analyse their atomic structure by observing them along the [0001] zone axis. It was found that in the best layers, where their density is below 1010cm-2, the threading dislocations bear two atomic configurations with 8 atom cycles or 5/7 rings along their line. In highly defective layers, large angle boundaries have been observed and additional 4 atom ring cores have been found.

When inversion domains are present, they are bounded by {10 0} facets and their boundaries were found either to exhibit Ga-Ga and N-N bonds or to be reconstructed.The two atomic configurations are related by a c/2 translation. Although {10 0} non inversion boundaries have been reported in GaN layers, in our samples, the only non inversion boundaries we have found to lie in {11 0} lattice planes. A thourough investigation has shown that they are prismatic faults and two atomic configurations have been observed, they have 1/2 $< 101 >$ and 1/6 $< 203 >$ displacement vectors respectively.

The {11 0} stacking faults have been found to easily fold from the prismatic to the basal planes and to originate from surface step in case of growth on (0001) SiC. The formation of inversion domains has been shown to minimize the misfit along the c axis in case of nanometric steps network at the (0001) sapphire surface.

TEM assessment of structural defects and nucleation sources within epitaxial GaN

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Abstract

There is continued need to gain improved understanding of the nature of crystallographic defects within semiconductors, to identify (and thereby control and/or eliminate) the reasons for defect nucleation and to ascertain the fine scale association of structural defects with material (opto)electronic recombination activity. Accordingly, we illustrate how complementary electron microscopical techniques can be used to reveal the atomic structure and formation process of

{11-20} prismatic stacking faults within MBE grown GaN; and confirm the precise nature of nucleation events responsible for the formation of inversion domains within homoepitaxial GaN grown by CVD. It is evident that complete understanding of the nature of structural

defects within GaN can only come about from a combined structural, optical and electronic study of defects combined with theoretical calculation. In this context, we comment on the development of the technique of scanning transmission electron beam induced conductivity (STEBIC) and comment on its applicability to investigate material recombination activity within the GaN system.

Session 10: Extended defects in III-Vs continued

Chair: Pierre Ruterana

The structure, growth and opto-electronic properties of defects in InGaN/AlGaN/GaN layers

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Abstract

Light emitting devices based on GaNInGaN/AlGaN layers have proved enormously successful. Yet this success is surprising since the active layers often contain threading defects at densities up to 109 cm^{-2}, orders of magnitude higher than acceptable in most other semiconductor devices. To understand this problem, we have used transmission electron microscopy (TEM) to analyse the defects and cathodoluminescence in the scanning electron microscope (SEMCL) to determine their light emitting properties. Using TEM we have analysed the structure of dislocations, nanopipes (shown to be screw dislocations) and inversion domains. The talk will illustrate some of these results and comment on the growth mechanisms.

In GaN/InGaN/AlGaN structures, high layer strains can occur with pseudomorphism persisting to much greater thicknesses than expected from equilibrium theory. This can be ascribed to the absence of shear stress on the basal slip plane. Recent work is described in which misfit dislocations lying in the basal plane are generated in AlGaN/GaN layers and in lateral-overgrown GaN in regions where shear stresses are present.

SEMCL studies have confirmed that defects in GaN structures act as non-radiative recombination centres but that carrier diffusion lengths are typically much less than in other semiconductors. The talk will illustrate some recent work in which we have mapped luminescence around individual defects in InGaN/GaN structures.

Role of dislocation walls on the free carrier mobility collapse in GaN

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Abstract

It is experimentally known that the free carrier mobility versus dopant density in GaN grown by MOVPE on sapphire substrates experiences a particular behaviour which consists in the appearance of a sharp transition separating a low from a large mobility range as soon as the carrier density exceeds a critical value (about 5x1017 cm^{-3} in our samples). In the large mobility range, the carrier density may be described, using standard transport calculations while we show that the low value range cannot be theoretically recovered even when considering the various scattering mechanisms associated with a large density of dislocations.

In the particular case of bulk GaN grown by MOVPE on sapphire substrates, TEM observations indicate that, mainly, dislocations are generally arranged in walls.

In this contribution, we show that the particular mobility behaviour is controlled by the presence of such dislocation walls and results from a transition between a barrier-controlled mobility and a pure-diffusion-process-controlled mobility because of screening effects which reflect into the following mechanism: as long as the band bending introduced by neighbouring charged dislocations engaged in the walls overlaps, dislocation walls act as an electronic barriers. However, increasing the carrier density (and therefore the screening effects) leads to a transition between overlapping dislocations potentials (barriers) and individual dislocations (pure diffusion range).

A theoretical model based on screening properties has been constructed for the description of such a transition behaviour of dislocation walls. When introduced in the standard relaxation time description of transport phenomena, it allows us to perfectly reproduce the experimental data and finally to get an estimate of the "mean" position of the dislocation energy states which appear to be centred at about 150 meV under the conduction band.

In-situ transmission electron microscopy studies of defect formation and dislocation interactions in semiconductor materials

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Abstract

Real time observations of the SiGe / Si (001) crystal growth process within the objective lens of the transmission electron microscope permit investigation of the interaction between threading and misfit dislocations. We find that in addition to the anticipated long range blocking of dislocations due to inter-dislocation forces, a new short range mechanism exerts

a more significant effect on strain relaxation. Computational simulations show that this reactive blocking mechanism occurs when dislocations with parallel Burgers vectors re-connect.

In other work, in-situ annealing of stress-free single crystal GaN films allows investigation of the effect of nitrogen desorption on defect formation. Upon reaching the desorption temperature of 950°C, nanopipes form selectively along the cores of screw axis dislocations. Dislocations with mixed character propagate within the basal plane of the film along well defined type directions if under stress, and leave a hollow tube in their wake. Dislocations of pure edge character are not affected. Because GaN growth via chemical vapor deposition requires temperatures in excess of 950°C to decompose elemental nitrogen from the carrier gas, nanopipe formation during crystal growth may be unavoidable. Additionally, these results indicate that light element desorption and dislocation motion may occur simultaneously in wide band-gap semiconductors.

Session 11: Extended defects in III-V compounds continued

Chair: David Cherns

Dislocations in GaN

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Abstract

We present our computational results for several types of line defects in both hexagonal and cubic GaN. Most investigated stoichiometric extended defects in hexagonal GaN do not induce deep acceptor states and thus cannot be responsible for the yellow luminescence. However it is shown that electrically active defects in particular gallium vacancies and oxygen related defect complexes are trapped at the stress field of the dislocations. Recent calculations for cubic GaN find the ideal stoichiometric 60°dislocation to be electrically active. This dislocation is also likely to trap impurities at its core.

Deformation Dislocations in GaN

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Abstract

GaN and its alloys constitute wide bandgap semiconductors that show considerable promise for optoelectronic applications. Unlike growth dislocations that have been extensively studied in these materials, there has been very little work on deformation-induced dislocations. Thus, there is a paucity of information on the behavior and microstructure of deformed GaN mainly because bulk crystals of this material are not readily available. Using the technique of hydride phase vapor epitaxy (HPVE), it is possible to grow relatively thick single crystal GaN films (with a thickness of 100 μm or more). We have employed such HPVE GaN crystals and investigated their indentation behavior as a function of temperature and load. Various faces of an HPVE GaN crystal, e.g. parallel to basal as well as prism planes, were deformed by Vickers indentation over a range of temperatures from 25 to 1200°C. Following the indentations, the defect microstructure of the deformed crystals was investigated by transmission electron microscopy (TEM). These results will be discussed and compared with deformation-induced dislocations in other semiconductors.

Session 12: Extended defects in III-V compounds continued

Chair: John Northrup

Stacking fault effects in Si doped GaAs

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Abstract

We investigate the electronic perturbation caused by stacking faults in Si doped GaAs. The ab initio calculations were performed within density functional Theory in the local density approximation. Norm-conserving pseudopotentials were used to model the ionic potential and the valence electron wavefunctions were expanded in a plane-wave basis set. Our calculations show that the main changes in the electronic energy levels in pure GaAs due to the presence of stacking faults occur at the top of valence band, introducing levels inside the band gap. Si in the Ga site at the stacking fault core is energetically favorable

by 0.12 eV/impurity as compared to the Si at the crystal-like environment. The Si impurity in the negative charge state also is favorable at the fault by 0.19 eV,and it can occupy a metastable interstitial position, close to the Ga substitutional position. At that metastable position the Si impurity level enters in the gap, becoming a deep level, working similarly to the DX-Center, but with considerably smaller lattice relaxation.

Ab initio study of the effect of doping on stacking faults in GaN

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Abstract

Recent TEM studies have shown that silicon doping has a strong influence on the defect structure of wurtzite GaN [1]. In particular the density of basal plane stacking faults is found to increase with silicon doping whereas the density dislocations reaching the free surface is reduced. The reduction in dislocation density is thought to be directly related to the presence of the stacking faults.

In this study we investigate the relationship between impurity concentrations and stacking fault densities in GaN by calculating the stacking fault energy as a function of impurity doping. The calculations are based on density functional theory in the local density approximation and employ norm conserving non-local pseudopotentials. For the case of silicon, the stacking fault energy reduces with increasing silicon concentration in agreement with experimental observations of higher stacking fault densities in silicon doped GaN compared to undoped GaN. The result is explained in terms of an increase in the degree of covalent bonding as silicon is incorporated into the lattice and a reduction in the Mulliken charges on the atoms. We propose that Mulliken charges can be used to predict how any substitutional impurity will influence the stacking fault formation energy. This proposition is checked by investigating the stacking fault energy and the bonding characteristics in GaN doped with magnesium, carbon and indium.

[1] S. I. Molina, A. M. Sanchez, F. J. Pacheco, R. Garcia, M. A. Sanchez-Garcia, F. J. Sanchez and E. Calleja, Appl. Phys. Lett. 74, 3362 (1999).

On the anisotropic microhardness and crack propagation in epitaxially grown GaN films

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Abstract

The anisotropic character of microhardness, in cubic and hexagonal GaN films epitaxially grown on SiC and on sapphire respectively, is investigated. A series of Vickers indentations demonstrate anisotropic indentation induced crack propagation in cubic GaN while in the hexagonal material no cracks are formed for idendations with the same load. Directions of easy crack propagation are observed. A series of Knoop indentations are conducted in order to inspect the possible microhardness orientation dependence relative to the main crystallographic directions of films. The measurements reveal an orientation dependence of microhardness only in hexagonal GaN films. The indentations are made with an angular interval of five degrees and the microhardness - orientation curve is obtained. The curve has a periodicity close to sixty degrees.

Work supported by EU RTN contract HPRN-CT-2000-00040

Electron microscopy study of dislocation bending in ELO-GaN layers grown by hydride vapour phase epitaxy

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Abstract

Transmission and scanning electron microscopy studies of defects in GaN layers grown by selective epitaxy are reported. High defects densities in thick GaN layers are usually observed due to the lattice and thermal mismatches between GaN and the currently used growth substrates. This has a strong influence on the quality of GaN based devices. Hydride vapour phase epitaxy (HVPE) in combination with epitaxial lateral overgrowth (ELO) has shown to be very promising in obtaining high quality GaN layers on sapphire with low dislocations density, high growth rates and good selectivity. Metal organic vapour phase epitaxy (MOVPE)-GaN(0001)/sapphire(0001) layers are patterned with SiO2 stripes aligned along ·1-100Ò direction of GaN. Triangular GaN stripes of 15mm height are formed during the growth that is performed using hydrogen/nitrogen mixtures as carrier gas. The resulting rough surface is subsequently flattened using pure nitrogen. Density of threading dislocations is 1x1010cm^{-2} in MOVPE starting layer. The dislocation density in the upper layers can be reduced by fast lateral growth. Before coalescence of the selectively grown regions, three types of dislocations are identified: edge, screw and mixed dislocations. In the region between SiO2 mask they are bent in horizontal directions. Different bending behaviour for different types of dislocations is observed. Upper layers have dislocations density less than 1x107cm^{-2} and they are free from vertically propagating dislocations. Further overgrowth to the 40mm thick layers and the cooling process from the 1050°C growth temperature induces formation of new defects.

Analysis of strain in the {11 0} prismatic fault in GaN using digital processing of HRTEM

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Abstract

Using the geometric phase method and measurement of dislocation core distribution a quantitative analysis of the contrast exhibited by [0001] HRTEM images of the {11-20} prismatic stacking fault in GaN was carried out. Such analysis allows to determine precisely the displacement vector and to locate any additional defect inside the boundary such as steps, dislocations, etc.

It is found that in many cases, dislocations are pinned inside the boundary. They appear to be always associated as dislocation dipoles with stress fields, which locally modify the atomic structure in the boundary plane. For fully relaxed segments, perfect matching between experimental and simulated images based on Drum model was obtained. When stress fields are present, the deviation of the boundary atomic structure from the theoretical models is significant.

The occurrence of such dipole seems to be connected to the growth mechanisms of the GaN film, which is mosaic and gives rise to rotated islands.

Saturday 22nd July
Session 13: Extended defects in group IV elements and compounds

Chair: t.b.a.

Plastic deformation of single crystals of C_{60} AND C_{70}

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Yu.A. Ossipyan, N.S.Sidorov, E.A.Steinman
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Abstract

In this work method of selective etching has been developed to reveal dislocations and other defects in C_{60} single crystals. The character of them real structure alterations due to plastic deformation caused by microindentation of the surface has been studied. The crystallography and specific features of the dislocation glide and crack formation in C_{60} crystals have been analysed.

The results of strain-stress measurements made on C_{60} single crystals and the photoluminescence (PL) spectra of plastically deformed samples are reported. A hardening of samples with increase of the deformation temperature from 20°C to 300°C was observed together with a strong enhancement of some defect related lines in PL spectra. We suppose that appearance of covalently bonded C_{60} molecules at dislocations is a possible reason for that.

The mechanisms of plastic deformation of C_{70} single crystals during microindentation have been studied with the optical microscopy. It is shown that the plastic deformation goes by the formation and motion of dislocations. The dislocation slip systems are revealed. The anisotropy of the hardness caused by the features of the dislocation glide in C_{70} has been found.

Extended Defects in Diamond under the Electron Microscope

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Abstract

Diamond can be regarded as a (very) large bandgap semi-conductor. The addition of electron spectrometry to the electron microscope has enabled the direct and indirect gaps of such materials to be measured in the electron microscope. But more importantly, the chemical and electronic properties of the defects can be determined from the electron energy loss spectrum, excited locally at a chosen defect.

Several examples are given:

1. The state of aggregation of nitrogen donors in diamond has been greatly clarified. It has been shown how the formation of nitrogen pairs, triplets and fours from monatomic substitutional nitrogen leads to the precipitation of carbon intersitials in the form of platelets.

2. In the case of deposited films of the diamond like carbons, one can measure the state of bonding, and correlate that with properties and depostion conditions. One finds a strong correlation between type of bonding and density, different for hydrogen-containing films and 'pure' carbons.

It is hoped that the analogies with silicon can be discussed.

Small aggregates of interstitials and models for platelets in diamond

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S. Öberg
Department of Mathematics, University of Lulea, Sweden

Abstract

Recent experiment and modelling has shed light on the structure of small numbers of interstitials in diamond. Electron paramagnetic resonance has been used to identify the structure of the isolated interstitial as well as aggregates of two or three. However, large aggregates of interstitials form structures refered to as platelets, for which the detailed structure is less well understood. For example, it was believed that nitrogen constituted a substantial proportion of the platelet, but now it is generally accepted that they are largely native in nature.

We present the results of optimising a number of models for small aggregates of interstitials and platelets in diamond. Using a periodic system, we have established the relative energies for different arrangements of atoms based loosely around the platelet model due to Humble [1]. These amount to interstitial precipitates.

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Theory of dislocations in diamond and interactions with H

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Abstract

Dislocations in silicon were shown at the last EDS meeting to be profoundly affected by a hydrogen plasma. Subject to a long pre-treatment with H plasma, the activation energy for motion could drop from its normal 2.2 eV to 1.2 eV [1]. First principles calculations based on the movement of hydrogenated solitons on the 90° partial reproduce this behaviour [2].

Since low pressure growth of diamond and hard, amorphous forms of carbon often occurs largely in the presence of a highly energetic H plasma, it begs the question whether a similar phenomenon can be observed in dislocations in diamond (and by extension, structural relaxation within dense amorphous carbons).

Repeating the calculations for diamond, we confirm that, inasmuch as the same processes are rate determining for dislocation motion in diamond, the same effect should be observable in principle, and that, by and large, most energies of formation and migration scale with those in silicon as the ratio of the cohesive energies for silicon and diamond.

[1] Y. Yamashita, F. Jyobe, Y. Kamiura and K. Maeda, Phys. Stat. Sol. (a) 171 (1999) 27

[2] C.P.Ewels, S.Leoni, M.I. Heggie, P.Jemmer and E.Hernandez, Phys. Rev. Lett. 84 (2000) 690

POSTERS

1. S. Dassonneville, A. Amokrane, Jean-Louis Farvacque, B.Sieber, B. Beaumont, V. Bousquet, P. Gibart, J-D. Ganiere, and K. Leifer
"Defect diffusion and strain relaxation in epitaxial GaN laterally overgrown on (0001) sapphire under low energy electron beam irradiation"

2. Anouck Riviere-Jerome, C. Levade, G. Vanderschaeve, I. Percheron-Garcon, B. Forgerit
"A TEM study of slip lines in power MOS devices"

3. Jun. Chen, P. Ruterana and G. Nouet
"An atomistic study of the atomic configurations of the edge threading dislocation in GaN using an empirical potential"

4. Suzel Lavagne, C. Levade,G. Vanderschaeve, J. Cristou, E. Tournie, JP. Faurie
"TEM study of crystal defects in ZnSe/GaAs (001) epilayers"

5. P. Kominou, G. Nouet, Th. Kehagias, G. Dimitrakopulos, Pierre. Ruterana, Th. Karakostas
"Interfacial dislocations in TiN/GaN thin films"

6. G. De Saint Jores, Pierre Ruterana
Microstructure and inteface analysis in ELO over AlN grown on(0001) SiC by HVPE"

7. Pierre Ruterana, F. Omnes, D. Schenk, B. Damilano, N. Gandjean and J. Massies
"In composition and strain relaxation inside InGaN epitaxial layers"

8. V. Potin, Pierre Ruterana and G. Nouet
"Analysis of stacking faults in AlN/GaN layers grown on saphhire substrate"

9. F. Degave, Pierre Ruterana and G. Nouet
"Microstructure of GaN films grown on (0001) sapphire by CBE as related to buffer growth conditions"

10. M. Legros, A. Jacques and Amand George
"Cyclic deformation behaviour and dislocation structures of silicon single crystals"

11 F.Riedel, Th.Kietzke, Wolfgang Schroeter
"DLTS measurements on nano-sized NiSi2 and Cu3Si precipitates in silicon"

12. Slawomir Kret, P. Dluzewski and P. Dluzewski
"Measurement of dislocation core distribution by digital processing of HRTEM micrographs: new utility for studying defects"

13. Ichiro Yonenaga, T. Hoshi and A. Usui
"High Temperature Hardness of Bulk Single Crystal GaN"

14. Ichiro Yonenaga and T.Suzuki
"Cross-slip in GaAs and InP at elevated temperatures"

15. Samantha Jenkins, C P. Ewels, and M. I. Heggie
"Analysis of bonding for the interaction of hydrogen with dislocations in diamond"

16. Simon Scarle, A. Mainwood, S.Leoni, C. P. Ewels and M. I. Heggie

"Modelling of impurities and dislocations in SiGe alloys"

17. Cesare Frigeri, J.L. Weyher and J. Jimenez
"On the absence of As decoration precipitates in Te-doped GaAs"

Defect diffusion and strain relaxation in epitaxial GaN laterally overgrown (0001) sapphire under low energy electron beam irradiation

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Abstract

Epitaxial lateral overgrowth of GaN on stripes opened in SiO2 or SiN mask (ELOG), leads to a reduction of the dislocation density. Thus, ELOG specimens are good candidates for studying independently the evolutions of the background (bulk) luminescence and of the dislocation recombination activity. The results we present in this paper have been obtained at 90 K, 10 keV and 10 nA, by plan view cathodoluminescence in a scanning electron microscope (SEM/CL). The ELOG samples have been grown by organometallic vapor phase epitaxy in a vertical reactor operating at atmospheric pressure. The overgrowth of GaN has been undertaken with a two-step process or with the addition of magnesium.

We show that the dislocations are efficient non radiative recombination centers since they are imaged individually with intrinsic (UV) and extrinsic (yellow and blue) luminescence bands. Their CL contrast is in the range 20-50%. Such large values associated with the CL images evidence that the dislocations are decorated and surrounded by impurities.

Electron beam irradiation leads to a broadening and a red-shift of the UV luminescence band. The red-shift increases with the compressive strain initially present in the epilayer. When the sample contains magnesium, the UV luminescence is, after 40 min of e-beam irradiation, about twice its initial value. When the sample does not contain magnesium, the UV luminescence decreases by a factor 2 within the same irradiation time. When the irradiation is performed in the spot mode, a dot surrounded by a circular halo appears, which shows that diffusion of point defects has occurred. We suggest that the dot is a tangle of dislocation loops which have been formed by the association of non radiative point defects. The redistribution of point defects within the crystal is also evidenced by a quantitative analysis of CL images of extended defects: after e-beam irradiation, i) the dislocations are cleaner (their CL image is thinner), and sometimes less electrically active, ii) the luminescence of coalescence boundaries is recovered.

A TEM study of slip lines in power MOS devices

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Abstract

During the different steps of integrated circuits manufacturing, the silicon wafers are subjected to mechanical and thermal stress. Stress relaxation occurs via slip dislocation generation and propagation, degrading electrical characteristics of the devices. We present here the results of a TEM analysis on defects in slip bands (whose traces at wafer surface are called slip lines) in devices for automotive applications. Two different samples types were investigated : wafers taken after the epitaxy step and wafers that went through the whole process, so containing operational devices.

Surface characterization by means of AFM (tapping mode) and selective chemical etching (Sirtl etch) revealed that slip bands contain an inhomogeneous density of dislocations. TEM analysis showed that the extremity of a slip band contains a high density of dislocations, inducing a large strain field in the crystal. The characteristic features of the dislocations structures (cusps and elongated dipoles on dislocations lines, presence of small dislocation loops in the slip band) will be discussed. It is suggested that dislocations interact with small defect clusters during their movement. The similarities and difference between the two kinds of samples will be emphasized.

An atomistic study of the atomic configurations of the edge threading dislocation in GaN using an empirical potential

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Abstract

High resolution TEM has recently shown that three atomic configurations of edge threading dislocations can exist in GaN. They are made of 4, 5/7 and 8 atom cycles respectively mostly inside [0001] grain boundaries. Previous observations and ab-initio calculations have pointed out that the reconstruction of the 8 atom cycles configuration could explain the high optical performance of GaN layers containing 1010 cm^{-2} dislocations. These configurations may have different behaviour, for example, the 5/7 which is expected to contain N-N and Ga-Ga bonds and the 4 atom core is highly distorted. In this work, we have used a modified Stillinger-Weber potential in order to investigate these configurations. We will discuss their structural stability inside good quality layers and in the high angle grain boundaries.

TEM study of crystal defects in ZnSe/GaAs (001) epilayers

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Abstract

The performance of light emitting optical devices based on II-VI semiconductors is greatly dependent on the density of the crystal defects in the material and on their dynamics under operation.

ZnSe thin films grown on (001)GaAs substrate by molecular beam epitaxy to a thickness of 2500Å have been studied by transmission electron microscopy (TEM). The purpose of this investigation is the characterisation of as grown crystal defects prior to a study of their dynamics by in situ straining and heating experiments in TEM.

Three types of structural defects have been observed:

· Triangular shaped stacking faults in the layer, with the apex close to the interface, either isolated or by pair. They are bounded by two different Shockley dislocations.

· Stacking faults generated from the free surface of ZnSe epilayer by movement of a Shockley half loop. These defects glide in {111} plane under the stress. Reaching the interface, they line up to $< 110 >$ directions.

· An array of perfect misfit dislocations. Their Burgers vectors are inclined to the interface. Most of them lie on$< 310 >$directions, only a few are parallel to$< 110 >$. Their direction can suddenly change from $< 310 >$ towards $< 110 >$. Furthermore interactions with stacking faults are noticed.

Interfacial dislocations in TiN/GaN thin films

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Abstract

Thin films of stoichiometric cubic TiN for ohmic contact formation are directly deposited, by rf magnetron sputtering at room temperature, on (0001) surfaces of GaN epilayers grown on c-plane sapphire. Chemical etching and in-situ dry etching of the free GaN surface allows an epitaxial growth of the deposited TiN films as revealed by High Resolution Electron Microscopy observations (HREM). Taking into account the experimentally determined orientation relationship of the two structures: (0001)GaN//(111)TiN, [11-20]GaN//[-110]TiN, three families of dislocations are expected in the interface plane to accommodate the misfit

(˜5.8%). The circuit mapping technique is used to analyse the dislocation content on HREM images. This gives a result 1/2[10-10]GaN or 1/4[211]TiN for the edge component of their Burgers vector with a spacing of 4.1 nm.

Microstructure and interface analysis In ELO GaN over AlN grown on (0001) SiC by HVPE

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Centre de Recherche sur l' Hétéroépitaxie et ses Applications (CRHEA, UPR 10 CNRS), rue Bernard Gregory Sophia-Antipolis, Valbonne F-06560

Abstract

ELO has now demonstrated the possibility to reduce the density of threading dislocations by orders of magnitude in GaN grown on sapphire. It has been shown that in conventional growth, no extensive difference exists in the densities of defects inside layers grown on sapphire or SiC, notwithstanding the difference in lattice mismatch : 16% and 3.5% respectively. The use of AlN buffers on SiC allows to decrease the misfit to 2.4%.

In this work, we have investigated the microstructure of ELO GaN on HVPE AlN, in order to determine the mechanism which underlies the defects formation. We studied the first stages of GaN ELO and we present the results on the kind of defects in AlN and their possible transmission or disappearance at the AlN/GaN interface. As the windows had a cylindrical shape, it was possible to analyse the type of threading dislocations and a different behavior was found between a and c type dislocations.

In Composition and strain relaxation inside InGaN epitaxial layers

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Abstract

Independently of the growth method, recent studies show that the InGaN layers are quite difficult to grow when the In composition increases. Due to the intrinsic properties, InN and GaN exhibit a miscibility gap, moreover their stability and growth temperatures are rather different. As is now quite understood, a number of typical defects form inside the ternary layers. Among them, V shape pits tend to appear at In concentrations as low as 2-3% if no special care is taken. Their density and depth increase with the In composition. We have found that the critical thickness for misfit dislocations generation at the interfaces with the ternary layers is multiplied by a factor of two in layers containing these defects. It was also noticed that they tend to be connected to threading dislocations with a screw character. In these strained layers, the growth of quantum wells allowed us to point out that two typical relaxation mechanims take place. They are the well known bending into the interface of existing dislocations which propagate from the underlying layer and the formation of surface loops followed by their glide into the interface.

Analysis of stacking faults in AlN/GaN layers grown on sapphire substrate

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Abstract

Three types of basal stacking faults are reported to exist in the hexagonal close-packed structure: two intrinsic faults I1 and I2 (with vectors equal to $1/6 < 20-23 >$ and $1/3 < 10-10 >$, respectively) and the extrinsic fault E (b = In GaN/AlN layers, these faults correspond to the insertion of one, two or three cubic stacking sequences in the wurtzite structure. We have studied the microstructure of AlN/GaN layers grown by metalorganic chemical vapor deposition technique on vicinal (0001) sapphire substrate. Using high resolution electron microscopy, we have investigated the layers near the interface with the substrate. Several I1 and I2 stacking faults were observed: some of them have large extension. Nanometric areas of faulted sequences were found to be due to simple shear during growth, they correspond mostly to I2 closed loops. However more complex configurations associated with dislocation reactions and/or climb have been observed.

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Cyclic deformation behaviour and dislocation structures of silicon single crystals

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Abstract

Si single crystals oriented for single slip were cyclically deformed in tension/ compression in order to study the dislocation behaviour in fatigue of fcc materials with large Peierls potential.

Tests were performed, with plastic strain control, between 1123 K and 1173 K, at a shear strain rate of 3 ´10-4 s-1. Saturation of the peak stress was reached after about 104 cycles for a plastic strain amplitude per cycle of 4 ´10-3.

TEM observations in saturated samples revealed persistent slip bands, with the typical ladder structures.

DLTS measurements on nano-sized NiSi2- and Cu3Si precipitates in silicon

F.Riedel, Th.Kietzke, Wolgang Schröter

Abstract

We report results of a study of electrical properties of nano-sized nickel and copper silicide precipitates, respectively, in silicon by means of deep level transient spectroscopy (DLTS). These extended defects as-quenched originate deep bandlike states. This is revealed by the specific characteristics of the associated respective DLTS line. For NiSi2 platelets with diameters ranging from 10 to 140nm we investigated the dependence of DLTS line characterstics on platelet size. At small platelet size a dramatic increase of the line width is observed. Double DLTS measurements on nano-sized Cu3Si and NiSi2 platelets are presented which allow to investigate the significant influence of the electric field in the space charge region of the Schottky contact on the emission of captured charge carriers from these extended defects.

Measurement of dislocation core distribution by digital processing of HRTEM micrographs: A new utility for studying defects

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Abstract

A new utility for studying extended defects and dislocation networks is proposed. The approach based upon the continuum theory of crystal defects is employed to digital image processing of high resolution transmission electron micrographs. The procedure starts with calculation of the lattice distortion field near dislocation cores by using the geometric phase method. Then, the dislocation core distribution (DCD) is recovered from the lattice distortion field. Such DCD takes non-zero values only in lattice disordered regions. The accuracy of this method is investigated by mathematical integration of dislocation field over core regions to find the components of Burgers vectors in the projection plane. The proposed method is free of topological problems and can be used to study spatial configurations of complex defects in large crystal areas.

This approach has been applied to investigate a network of misfit dislocations in the interfacial region of GaAs/ZnTe/CdTe heterostructure. The relation between atomic structure of misfit dislocation to calculated dislocation core distributions is discussed.

High Temperature Hardness of Bulk Single Crystal GaN

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Abstract

The hardness of single crystal GaN (gallium nitride) at elevated temperature is measured for the first time and compared with other semiconductors. Crack-free single crystals of 500 mm thickness with mirror-like surfaces were prepared by hydride vapor phase epitaxy with facet-initiated epitaxial lateral overgrowth. A Vickers indentation method was used to determine the hardness of GaN samples under an applied load of 0.5N in the temperature range 20 - 1200°C. The hardness is 10.8 GPa at room temperature, which is similar to those reported by Drory et al.[1] and Pirouz et al.[2]. Throughout the entire temperature range investigated, the hardness of GaN exhibits a gradual decrease from room temperature to 500°C, a plateau in the range from 500 to 1000°C, and subsequently a steep decrease. Such the temperature dependent tendency is similar to that of 6H-SiC and sapphire, with the similar hcp-based structure. It is found that GaN is harder than GaAs in the whole temperature range investigated and that at temperatures lower than 600°C the hardness of GaN is comparable to, or a little lower than that of Si. Up to about 1100°C, GaN keeps

its hardness, being harder than Si and GaAs. A high mechanical stability for GaN at high temperature is deduced.

References

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[2] M. H. Hong, P. Pirouz, P. M. Tavernier and D. R. Clarke, Mat. Res. Soc. Symp. Proc. 622 (2000) in press.

Cross-slip in GaAs and InP at elevated temperatures

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** *Institute of Industrial Science, University of Tokyo, Tokyo 106-8558, Japan*

Abstract

Slip lines on GaAs and InP crystals plastically deformed up to the lower yield point at temperatures around 700 K are compared with similar observations on Si. The slip lines in GaAs and InP differ from those in Si in two aspects: the primary slip lines are wavy and the non-primary slip lines are long and straight. The former are similar to those found in GaAs and InP crystals deformed at low temperatures (< 400 K), being common among III-V compounds, and suggests a glide motion of undissociated screw dislocations. The operation processes of the non-primary slips are discussed with an X-ray topographic analysis of GaAs.

Analysis of bonding for the interaction of hydrogen with dislocations in diamond with implications for diamond like carbon (D.L.C)

Samantha Jenkins, M. I. Heggie, and C.P.Ewels

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Abstract

In order to understand and hence control the growth and annealing of D.L.C we need to understand the mechanisms involved in structural rearrangement of the material.

We do this by studying dislocation cores which are regions of crystal where short range order is preserved (as it is in tetrahedral amorphous carbon, ta-C) but long range order is largely lost. The chemistry and physical properties of these dislocations are then studied, especially when modified by a hydrogen plasma.

Previous studies on silicon gave the correct activation energy (E = 1.2 eV) for dislocation motion in the presence of an H plasma[1]. We report first principle (DFT) modelling which shows the effect of the differences the chemical bonding between silicon and diamond. We quantify the bonding of metastable, saddle point and ground states occurring in dislocation motion by analysis of the charge densities.

[1] C.P.Ewels, S.Leoni, M.I. Heggie, P.Jemmer and E.Hernandez, Phys. Rev. Lett. l84(4) 690-693.

Modelling of impurities and dislocations in SiGe alloys

Simon Scarle[1], A. Mainwood[2], S.Leoni[1], C. P. Ewels[1],
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Abstract

We present results on the segregation energies from first principles of Ge to surface and to dislocation sites (the 90 ° partial), finding energies as large as 0.25 eV. We also present an analysis based on valence force potentials of the changes in vibrational frequencies with alloying and doping in SiGe alloys.

7 General Job Announcements

Postdoctoral Position

Theoretical Magnetism

Physics Department
University of Warwick, UK

A three-year post-doctoral research position is available from 1 January 2001 to work in the electronic structure group of *Dr Julie Staunton* on a project to develop a theory for the temperature dependence of magnetic anisotropy (MCA) in bulk and film samples of magnetic metals and alloys. The variation of MCA of binary and ternary transition metal alloys with both compositional order and tetragonal strain is also to be studied and the key electronic factors extracted to obtain a guide as to how to increase and decrease these quantities. It is hoped that 'first-principles' relativistic electronic structure basis of this work will make it relevant to experimental work using magnetic X-ray scattering, magneto-optics, ferromagnetic resonance, neutron spin polarised reflection measurements etc. Extraction of temperature dependent anisotropy parameters from the work should be useful in micromagnetic modelling and magnetic material design. The computational codes upon which this work will be based have a natural coarse-grained parallelism and are run on a number of platforms including the Cray T3E at CSAR, Manchester.

The project is funded by the Engineering and Physical Sciences Research Council of the UK and the salary for the postdoctoral position is on the RA1A scale (currently 18185 - 23651 UK pounds, pay award pending).

Candidates for this post must have (or expect to obtain soon) a Ph.D in theoretical or computational condensed matter physics or related discipline. Experience with electronic structure calculations and parallel computers is desirable.

Enquiries and applications, the latter including curriculum vitae and the names (and e-mails) of at least two referees should be sent to

Dr.Julie Staunton
E-mail address: j.b.staunton@warwick.ac.uk.
Postal address: Department of Physics, University of Warwick, Coventry, CV4 7AL, UK
Tel: +44 24 7652 3381; Fax: +44 24 7669 2016

Further information about the group including its recent publications can be found at
http://www.warwick.ac.uk/ phrjz

POSTDOCTORAL POSITION

Laboratoire des Solides Irradies
Ecole Polytechnique, 91128 Palaiseau (Paris), France

A postdoctoral position at the Laboratoire des Solides Irradies, Ecole Polytechnique, Palaiseau (Paris, France), in collaboration with Dr. Lucia Reining, is available starting from now.

The position is for two or three years (to be discussed), with the possibility of renewal for up to June 2004. It is financed by the European Community through a RTN network. To be eligible for an Network-funded appointment the applicant must satisfy the EU's criteria which are, in brief:

* aged 35 years or less (with certain exceptions)
a citizen of a member state of the European Union or a state associated with the Fifth Framework Programme (Bulgaria, Republic of Cyprus, Czech Republic, Estonia, Hungary, Latvia, Lithuania, Poland, Romania, Slovakia, Slovenia, Iceland, Liechtenstein, Norway, Israel. Malta, Turkey ad Switzerland maybe from 2001)
resident and working outside the proposed host country for more than 12 months of the last two years.

The research will be part of the ongoing collaborations within this network, "NANOPHASE: Nanoscale photon absorption and spectroscopy with electrons." NANOPHASE is a new Research Training Network, approved for funding by the European Union. The overall topic of the Network is the theory of nanometre-scale structures - atomic clusters, quantum dots on surfaces or embedded in materials, quantum wires, and molecules adsorbed on surfaces - and the spectroscopic processes that can be used to characterise those structures, their electronic and optical properties, and their growth. These will be studied using fundamental theory and state-of-the-art ab initio computer simulations. The seven NANOPHASE teams are: Fritz Haber Institute, Berlin; Friedrich Schiller University, Jena; Lund University; CNRS / Ecole Polytechnique, Paris; University of Rome "Tor Vergata"; University of Valladolid; University of York. (Please see also the network's home page

http://www-users.york.ac.uk/ rwg3/nanophase.html.)

In particular, the group in Palaiseau has been working during the last years in the field of one - and two-particles Green functions calculations (GW, excitons in optical absorption). These topics should be developped further, concerning both theory and numerics, preferably towards applications to defects. This work will include the determination, within DFT-LDA and using a plane-wave basis, of structural relaxations of point defects and clusters of defects in semiconductors and insulators, the calculation of the corresponding quasiparticle levels using the GW method, and absorption and luminescence spectra including excitonic effects.

If you wish to apply for this position, please send me your CV and any other information that you

judge important, as soon as possible. Thank you. Also, if you wish to have further information, please don't hesitate to contact me, or have a look at our web page:

http://www-drecam.cea.fr/lsi/groupe/theory.htm

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Ph.D. Position in Computational Physics

Peter Kratzer and Matthias Scheffler
Fritz-Haber-Institut der Max-Planck-Gesellschaft,
Faradayweg 4-6, D-14195 Berlin (Dahlem), Germany

Are you interested in working on the fundamental physics of nanoscale electronic components ? At the Theory Department of the Fritz-Haber-Institut, there is an opening for a Ph.D. position in a joint project with our experimental colleagues, funded by the German Research Council (DFG). We plan to do simulations of the structural and electronic properties of quantum dots (InAs embedded in GaAs). The main focus will be on the use of ab initio methods (density functional theory / tight-binding method) to investigate nanoscale systems in atomistic detail. For more information, visit our web page

`http://www.fhi-berlin.mpg.de/th/Highlights`

or send e-mail to

`kratzer@fhi-berlin.mpg.de`

.

The ideal candidate should

- enjoy working with computers
- be interested in programming/software development
- have some background knowledge in solid state physics/chemistry

Post-doctoral Position

Computational Materials Science Group
IBM Zurich Research Laboratory

At IBM Zurich Research Laboratory we have an opening for a post-doctoral position in the Computational Materials Science group - starting January 2001.

Candidates should have a PhD in either physics or chemistry, and be familiar with density-functional theory and computer simulations. The project he/she will be involved with, is the study of the electronic and structural properties of semiconductor/oxide interfaces.

Interested candidates should send their CV, list of publications, and the address of two referees to:

Dr Wanda Andreoni
IBM Research Laboratory Zurich
Saumerstrasse 4
CH-8803 Rueschlikon
e-mail: and@zurich.ibm.com

RESEARCH ASSOCIATE POSITION AT MILANO

University of Milano-Bicocca
Department of Materials Science

Position: Ricercatore INFM

Duration: 3 years, starting from November 2000, January 2001 at latest.

Requirements: PhD plus two years postdoctoral experience.

Expertises: Computational Solid State Physics by ab initio or tight binding methods/ Molecular Dynamics Simulations/Software skillness.

Activity: Prediction of transport and/or optical properties of silicon-based epitaxial nanostructures. Close connection to one new experimental growth facility.

Duties: Execution of one research project connected to the experimental growth facility. Supervision of PhD and PostDoc activities in the theory group.

Neat Salary: 2.5 Million Lire per month, 13 months per year.

For additional information, please contact:

Prof. Leo Miglio
Dipartimento di Scienza dei Materiali
della Universita' di Milano "Bicocca"
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Tel. +39.02.6448.5217
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EU Postdoctoral Fellowships
in Computer Simulation of Many-body Systems (2)
Departments of Physics and Mathematics, Trinity College Dublin

Applications are sought for two EU Development Host Postdoctoral Fellowships tenable for up to 2 years in the Departments of Physics and Mathematics at Trinity College Dublin. In accordance with the rules of this EU programme, the Fellows appointed will be expected to contribute their existing expertise in the areas of: Hubbard models applied to simulation of materials and Simulation techniques for analysis of risk and financial markets. One Fellow is required to work in the area of condensed matter simulation using finite size scaling techniques applied to Hubbard-type models for magnetic materials and one Fellow is required to apply lattice simulation techniques to analysis of risk and financial markets.

Salary : 36,000 Euro p.a.

Application forms and further particulars relating to this post may be obtained from:

Dr. C.H. Patterson
Department of Physics
Trinity College
Dublin 2
Republic of Ireland
Tel: +353-1-608-1468
Fax: +353-1-671-1759
e-mail:Charles.Patterson@tcd.ie

Information about the Departments may be found at:

http://www.tcd.ie

Trinity College is an Equal Opportunities Employer.

Postdoctoral Fellowship
in Electronic Structure of Manganites
Trinity College, Dublin

The electronic structure group at Trinity College has developed a method for computing exchange coupling parameters in magnetic oxide materials (manganites). The fellow will be expected to develop this work on manganites and extend it to cuprates; to develop a qualitative theory for the exchange coupling using analytical and numerical models and to calculate optical excitation spectra of these materials using many-body methods. The fellow will use generally available electronic structure codes (CRYSTAL, GAMESS) and a solid state many-body perturbation theory code under development at Trinity College.

Salary : 18,000 Irish pounds p.a.

Application forms and further particulars relating to this post may be obtained from:

Dr. C.H. Patterson
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Information about the Departments may be found at:

http://www.tcd.ie

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8 Abstracts

$M_{4,5}$ Resonant Raman Scattering with final 4p-4d holes in Te, La and Gd: trends of the many body effects

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Abstract

We present experimental results on Resonant Raman Scattering in Te, La and Gd with M5 and M4 excitation. The spectra show clearly the importance of the final state interaction between the configuration having one 4p hole and that having two 4d holes. The weight of the spectral region at higher transferred energies is very much dependent on Z and it is higher at low Z. Moreover, the sensitivity to the change of the excitation energy is quite different in the three cases, while the energy extension of the spectra is not very different in the three cases (typically 50-55 eV with M5 excitation). We show how these findings can be rationalized in a simple and expressive way by considering the interplay between all energy scales characteristic of the process. These are the multiplet splitting, the spin-orbit, the strength of the configuration interaction, and the energy separation between the two configurations.

(Scheduled for Phys. Rev. B, issue 15 September 2000)
Preprints available from: g.vanderlaan@dl.ac.uk

Catalysis and corrosion: The theoretical surface-science context

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Abstract

Numerous experiments in ultra-high vacuum as well as (T = 0 K, p = 0) theoretical studies on surfaces have been performed over the last decades in order to gain a better understanding of the mechanisms, which, for example, underlie the phenomena of catalysis and corrosion. Unfortunately, often the results achieved this way cannot be extrapolated *directly* to the technologically relevant situation of finite-temperature and high-pressure. Accordingly, modern surface science has realized that bridging the so-called pressure-gap (getting out of the vacuum) is the inevitable way to go. Of similar importance are studies in which the temperature is changed systematically (warming up and cooling down). Both aspects are being taken into account in recent experiments and *ab initio* calculations.

In this paper we stress that prejudice and lack of understanding of the molecular processes, which occur at surfaces and actuate catalysis and corrosion, are still significant, but we also demonstrate how synergetic effects between theory and experiment are leading to the next step, which is the development of *simple concepts* and *understanding* of the different modes of the interaction of chemisorbed species with surfaces. To a large extent this is being made possible by recent developments in theoretical methodology, which allow to extend the *ab initio* approach to poly-atomic complexes with 10,000 and more atoms, time-scales of seconds, and involved statistics (*i.e.*, starting from the self-consistent electronic structure) approach to poly-atomic complexes with 10,000 and more atoms, time-scales of seconds, and involved statistics (*e.g.*, *ab initio* molecular dynamics with 10,000 and more trajectories). In this paper we will

- sketch recent density-functional theory based hybrid methods, which bridge the length and time scales from those of electron orbitals to meso- and macroscopic proportions,
- present some key results on properties of surfaces, demonstrating their role in corrosion and heterogeneous catalysis, for example. In particular we discuss
  - the influence of the ambient gas phase on the surface structure and stoichiometry,
  - adsorbate phase transitions and thermal desorption, and
  - the role of atoms' dynamics and statistics for the surface chemical reactivity.

(submitted to: Surf. Sci.)
Contact person: Matthias Scheffler (scheffler@fhi-berlin.mpg.de)

One-dimensional spin-polarized quantum-wire states in Au on Ni(110)

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Abstract

Au chain structures have been prepared on Ni(110). Au6s,p-derived features in photoemission spectra are identified as quantum-wire states due to their strong dispersion along the chains and absence of dispersion perpendicular to the chains in agreement with our *ab initio* calculation of the electronic structure. Spin analysis reveals that the states have minority-spin character showing that the confinement of electrons in the chain structure depends on the electron spin.

(Phys. Rev. Lett. **85**, 2561 (2000))
Copy available from: s.bluegel@fz-juelich.de

Electronic and magnetic structure of the (001)-surfaces of V, Cr, and V/Cr

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Abstract

We investigate the magnetic and structural properties of the (001) surfaces of V, Cr, and one monolayer V on Cr in density-functional theory in the local spin-density and the generalized gradient approximation. For both exchange-correlation potentials the surface magnetic moment of Cr is very large (2.6 μ_B) and the V surface is nonmagnetic. One monolayer V on Cr exhibits also a large magnetic moment (2.1 μ_B) but reduces the Cr moment drastically. The importance ot the surface moment on the spin-density wave of Cr is discussed. While some of the discrepancies between theory and experiment are cured by the generalized gradient corrections, several difficulties remain.

(Accepted at Phys. Rev. B, Rapid Comm.)
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Stability of high-pressure phase in small Ge quantum dots from ab initio calculations

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Abstract

In order to control and tailor the properties of nanodots, it is essential to separate the effects of quantum confinement from those due to the surface, and to gain insight into the influence of preparation conditions on the dot physical properties. We address these issues for the case of small Ge clusters (1-3 nm), using a combination of empirical and first-principles molecular dynamics techniques. Our results show that over a wide temperature range the diamond structure is more stable than tetragonal, ST12-like structures for clusters containing more than 50 atoms; however, the magnitude of the energy difference between the two geometries is strongly dependent on the surface properties. Based on our structural data, we propose a mechanism which may be responsible for the formation of metastable ST12 clusters in vapor deposition experiments, by cold quenching of amorphous nanoparticles with unsaturated, reconstructed surfaces.

(Submitted to: Phys. Rev. Lett.)
Latex-file available from http://xxx.lanl.gov/abs/cond-mat/0008145

Quantum Monte Carlo Analysis of Exchange and Correlation in the Strongly Inhomogeneous Electron Gas

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Abstract

We use variational quantum Monte Carlo to calculate the density-functional exchange-correlation hole n_{xc}, the exchange-correlation energy density e_{xc}, and the total exchange-correlation energy E_{xc}, of several electron gas systems in which strong density inhomogeneities are induced by a cosine-wave potential. We compare our results with the local density approximation and the generalized gradient approximation. It is found that the nonlocal corrections to e_{xc} contain an energetically significant component, the magnitude, shape, and sign of which are controlled by the Laplacian of the electron density.

(Submitted to Phys. Rev. Lett.)
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The Spin-Wave Stiffness within DFT and the Ginzburg-Landau Functional

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Abstract

The stiffness constant of the stationary spin excitation is calculated employing density functional theory (DFT) and the phenomenological Ginzburg-Landau (GL) energy functional in a site form. The exchange parameter of the magnetic functional is estimated within the framework of the nearest neighbours intermolecular interaction and the energy gain of non-magnetic state per atom. The stiffness constant of Fe, Co and Ni metals is found based on the energy gain of spin excitation calculated numerically in the local spin density approximation by Moruzzi *et al.* [1] as well as by Kübler [2].The calculated stiffness constants are compared with other theoretical calculations and experimental data. The energy gain of [2] yields surprisingly accurate results of the stiffness constant. Our calculated stiffness constant of *bcc* Fe, *fcc* Co and *fcc* Ni are, respectively, 79, 131 and 144 [mRy bohr^2]. The experimental low temperature values [3] are, respectively, 82, 134 and 144 [mRy bohr^2].

[1] V.L. Moruzzi, J.F. Janak and A.R. Williams, *Calculated Electronic Properties of Metals*, Pergamon, New York 1978.

[2] J. Kübler, *Acta Phys. Polon.* A **97**, 165 (2000).

[3] K. Tajima, Y. Ishikawa, P.J. Webster, M.W. Stringfellow, D. Tocchetti and K.R.A. Zeabeck, *J. Phys. Soc. Jpn.* **43**, 483 (1977).

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Density-functional study of the adsorption of benzene on the (111),(100) and (110) surfaces of nickel

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Abstract

The adsorption of benzene on all three low-index surfaces of nickel has been studied using gradient-corrected density-functional calculations. Our technique is based on ultrasoft pseudopotentials, residuum minimization techniques for the calculation of the electronic ground-state and of the Hellmann-Feynman forces and stresses, and on a conjugate-gradient technique for the optimization of the atomic structure. The surfaces have been modeled by periodically repeated slabs with up to six-layer slabs, allowing for the relaxation of the uppermost layer. For Ni(100) and Ni(110) surfaces an adsorption with the center of the aromatic ring placed above the hollow position has been identified to be energetically most favourable, whereas for the Ni(111) surface adsorption in the bridge position results in slightly higher binding energies. Adsorption-induced distortions of the molecular geometry are found to be modest in all cases: the C−C bond distances are slightly elongated, but the differences in the bond-lengths never exceed 0.03 Å. The aromatic ring remains flat, but the H-atoms are tilted away from the surface of the substrate. We also present a detailed analysis of electronic structure of the adsorbate/substrate complex and of the charge-flow induced by the adsorption Our results are discussed in relation to recent experiments and other theoretical studies.

(Submitted to Surface Science)
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Ab-initio investigation of the adsorption of benzene in mordenite

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Abstract

The adsorption of benzene in pure-silica and acid mordenite has been investigated using density functional theory, both in the local density approximation and including generalized-gradient corrections to the exchange-correlation functional. Benzene acts as a test molecule for studying the interaction between an aromatic hydrocarbon and a zeolite. Different adsorption modes have been studied for several acid sites. All configurations have been optimized by minimizing the total energy with respect to all lattice parameters and to the atomic coordinates. The strength of the adsorption is directly correlated to the local structural distortion of the zeolitic framework, especially of the acid site. Distortions of the acid sites indicate the formation of new bonds due to adsorption. Only if strong adsorption occurs, the molecule itself is slightly deformed. Furthermore, an analysis of the differential charges has been performed, indicating substantial polarization effects for the acid site as well as for the molecule. Finally, the red-shift of the OH-stretching frequencies due to the adsorption has been calculated and is compared to experimental IR data.

(Submitted to JCP)

Preprints available from: Thomas.Demuth@univie.ac.at

Scanning tunneling spectra of impurities in the Fe (001) surface

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Abstract

We present ab-initio calculations of scanning tunneling spectra (STS) for the Fe (001) surface and for 3d impurities in this surface. The calculations are performed by the full-potential Korringa-Kohn-Rostoker (KKR) Green's function method and partly also by the Full potential Linearized Augmented Plane Wave (FLAPW) method. For the clean Fe(001) surface we demonstrate that the correct tunneling spectrum is only obtained in a full potential treatment while the atomic sphere approximation yields incorrect results. For 3d impurities in the surface layer new peaks appear in the spectra due to surface-like states localized on the impurity site. Our results can explain recent STM experiments on Cr impurities in the Fe (001) surface and predict that chemical identification is also possible for many other transition metal impurities.

(To appear in Phys. Rev. B, Oct 15 (2000))
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Fully unconstrained noncollinear magnetism within the PAW method

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Introduction

In recent years a great deal of effort has been focused on developing the so called "fully unconstrained" approach to noncollinear magnetism. This approach allows the magnetisation density within a material to be calculated as a continuous vector variable of position as opposed to using the atomic moment approximation (AMA) where a fixed quantisation direction is assumed for a volume filling sphere surrounding each atomic site i.e. the constrained approach. The motivation for a fully unconstrained approach is to allow the magnetisation density to be correctly treated in the interstitial regions between atomic sites. While many materials have well localised magnetisation densities for which the AMA is valid, others (including the spin spiral ground-states of rare earths, topologically frustrated systems such as triangular monolayers and Kagomé lattices, spin-glasses, materials containing domain walls and/or at finite temperatures) may exhibit a de-localised magnetisation density which is more appropriately treated with a fully unconstrained approach.

Oda *et al.* [1] were the first to implement such an approach within a plane-wave pseudopotential scheme. Both the atomic and magnetic structure were allowed to relax simultaneously and self-consistently. Their method was applied only to small Fe clusters, which have less symmetry constraints than the bulk thus making them good candidates for noncollinear magnetic arrangements. Ivanov and Antropov [2] developed a wavelet technique for calculating the electronic and noncollinear magnetic structures in the framework of spin-density functional theory again without imposing shape restrictions to the magnetisation density. Their preliminary report studied the spin-structures of H_3 and Cr_3 clusters.

In parallel with our efforts here in Vienna, Nordström and Singh [3], Asada *et al.* [4] and Kurz *et al.* [5] have concentrated on developing the method within the full-potential linearised

augmented plane-wave (FLAPW) formalism. The approach of Nordström and Singh [3] is fully unconstrained in the sense discussed above while that of Asada *et al.* [4] and Kurz *et al.* [5] is adapted to suit the film geometry for surfaces and open structures. This adaptation imposes a constraint. The magnetisation density is treated as a continuous vector field in the interstitial region and in vacuum, while inside each muffin-tin sphere they allow only a fixed spin-quantitation axes. Since in the FLAPW the muffin-tin spheres are significantly smaller than the volume filling atomic spheres this extra constraint is probably a reasonable one.

Our objective has been to implement a fully unconstrained approach within the projector augmented wave (PAW) method. The PAW approach [6, 7] is an all-electron method for electronic-structure, total-energy and force calculations which is closely related to the ultrasoft-pseudopotential technique [8, 9]. In the PAW approach, charge- and spin-densities are decomposed into pseudo- and compensation densities accounting for the difference between the pseudo- and all-electron densities (see Fig. 1). The pseudo-densities consist of a smooth part expressed in a plane-wave representation and localised compensation charges accounting for the violation of norm-conservation [8, 9]. To account for differences between pseudo- and all-electron densities radial support grids are used. For each of the atom-centred radial support-grids the spin-quantisation axis is fixed - in this respect our approach resembles the unconstrained noncollinear FLAPW technique used by Asada *et al.* [4] and Kurz *et al.* [5], but unlike to the FLAPW method, in the PAW approach the plane-wave description is not restricted to the interstitial region, but extends over the complete volume of the system. Hence variations of the magnetisation direction are allowed also within the augmentation spheres. Our method allows both the atomic and magnetic structures to relax simultaneously and selfconsistently. The algorithms have been implemented within the Vienna ab-initio simulation package (VASP [10]). Below we present only a brief summary of the noncollinear PAW formalism, for a detailed discussion we refer the reader to Hobbs *et al.* [11]. Our results for small metallic clusters derive from Ref. [11] while the results for Cr and Mn on Cu(111) substrates are detailed in Ref. [12].

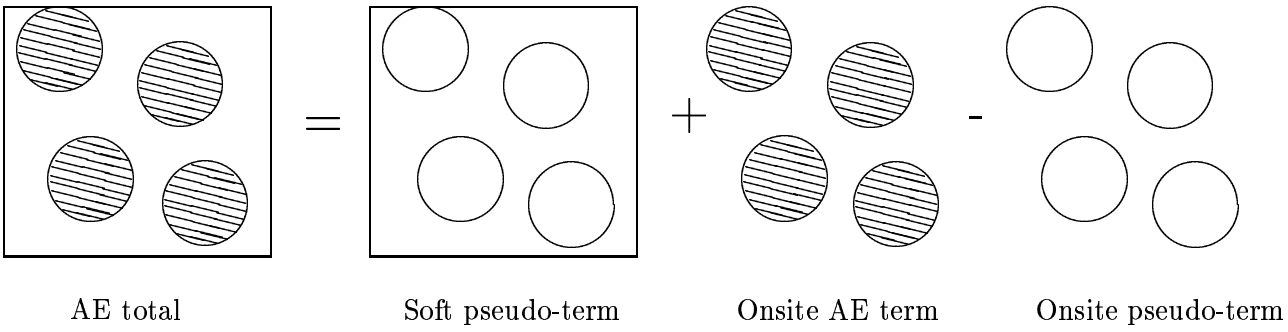

Figure 1: Illustration of the PAW approach. The AE charge density is constructed by modifying the total soft pseudo charge density by replacing the onsite pseudo-charge density with the onsite AE charge density. The same concept holds for wavefunctions, total energy and the Hamiltonian.

LSDF theory for noncollinear PAW

A generalisation of von Barth and Hedin's [13] local-spin-density-functional (LSDF) theory to noncollinear magnetism was first proposed by Kübler *et al.* [14, 15] within the framework of the

augmented-spherical-wave (ASW) method and the atomic-sphere-approximation. The effective single-particle equations for noncollinear magnets were derived by allowing the spin-quantisation axis to vary from site to site in crystalline systems. The orientation of the axis with respect to the reference frame is a property of the ground-state. They predicted well defined sets of directions for the spins, which are uncoupled from the crystal lattice unless spin-orbit coupling effects are included in the Hamiltonian (even though such effects are small in comparison to the spin-spin interactions).

Following Kübler *et al.* [14, 15], spin-polarised density functional theory is expressed in terms of a 2×2 density matrix with elements $n^{\alpha\beta}(\mathbf{r})$, where α and β refer to the spin indices. The electron density is then

$$\mathrm{Tr}\left[n^{\alpha\beta}(\mathbf{r})\right] \equiv n_{\mathrm{Tr}}(\mathbf{r}) = \sum_{\alpha} n^{\alpha\alpha}(\mathbf{r}). \tag{1}$$

The total density matrix may then be defined as

$$n^{\alpha\beta}(\mathbf{r}) = \left(n_{\mathrm{Tr}}(\mathbf{r})\delta_{\alpha\beta} + \vec{m}(\mathbf{r}) \cdot \vec{\sigma}^{\alpha\beta}\right)/2. \tag{2}$$

In addition, for the density matrix, we can make a transformation to the equivalent magnetisation density using the following formula [16]:

$$\vec{m}(\mathbf{r}) = \sum_{\alpha\beta} n^{\alpha\beta}(\mathbf{r}) \cdot \vec{\sigma}^{\alpha\beta}, \tag{3}$$

where $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli spin matrices. The exact Kohn-Sham density functional becomes (we use atomic units, $\hbar = m = e^2 = 1$)

$$E = \sum_{\alpha}\sum_{n} f_n \langle \Psi_n^{\alpha}| -\frac{1}{2}\Delta |\Psi_n^{\alpha}\rangle + E_H[n_{\mathrm{Tr}} + n_Z] + E_{xc}[n^{\alpha\beta}]. \tag{4}$$

$E_H[n_{\mathrm{Tr}} + n_Z]$ is the electrostatic energy of the electronic charge density n_{Tr} and the point charge densities of the nuclei n_Z and is defined by

$$E_H[\wp] = \frac{1}{2}\int\int \frac{\wp(\mathbf{r})\wp(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}d\mathbf{r}', \tag{5}$$

where $\wp = n_{\mathrm{Tr}} + n_Z$. $E_{xc}[n^{\alpha\beta}]$ is the electronic exchange-correlation energy and f_n are orbital occupation numbers. The exchange-correlation energy is not known in general, but only for a spin-polarised homogeneous electron gas with charge density n_{Tr} and magnetisation density $\vec{m}$. In the local-spin-density approximation $E_{xc}[n^{\alpha\beta}]$ is defined by:

$$E_{xc}[n^{\alpha\beta}] = \int n_{\mathrm{Tr}}(\mathbf{r})\epsilon_{xc}[n^{\alpha\beta}(\mathbf{r})]d\mathbf{r} = \int n_{\mathrm{Tr}}(\mathbf{r})\epsilon_{xc}[n_{\mathrm{Tr}}(\mathbf{r}), |\vec{m}(\mathbf{r})|]d\mathbf{r}. \tag{6}$$

The exchange-correlation functional leads to the nonmagnetic scalar exchange-correlation potential, v_{xc}, and to the magnetic exchange-correlation field $\vec{b}\left[n^{\alpha\beta}\right](\mathbf{r})$. The potential $\vec{b}\left[n^{\alpha\beta}\right](\mathbf{r})$ is parallel to the magnetisation density $\vec{m}(\mathbf{r})$ everywhere. The actual functional form of ϵ_{xc} can be parameterised in several ways (see Hobbs *et al.* [11]).

In the PAW method, the AE wavefunction Ψ_n^{α} is derived from the pseudo-wavefunction $\tilde{\Psi}_n^{\alpha}$ by means of a linear transformation [6]:

$$|\Psi_n^{\alpha}\rangle = |\tilde{\Psi}_n^{\alpha}\rangle + \sum_i (|\phi_i\rangle - |\tilde{\phi}_i\rangle)\langle\tilde{p}_i|\tilde{\Psi}_n^{\alpha}\rangle. \tag{7}$$

The pseudo-wavefunctions $\tilde{\Psi}_n^\alpha$ are the variational quantities. The index i is a shorthand for the atomic site $\mathbf{R}$, the angular momentum quantum numbers $L = l, m$ and an additional index k referring to the reference energy ϵ_{kl}. For noncollinear magnetism we define the pseudo-wavefunctions to consist of 2N eigenspinors, where N is the total number of eigenvalues. In our implementation, the pseudo-wavefunctions are expanded in reciprocal space into plane waves

$$\langle \mathbf{r}|\tilde{\Psi}_n^\alpha\rangle = \frac{1}{\Omega_r^{\frac{1}{2}}} \sum_{\mathbf{k}} C_{n\mathbf{k}}^\alpha(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{8}$$

where Ω_r is the volume of the Wigner-Seitz cell. The AE partial waves ϕ_i are obtained for a nonmagnetic reference atom, the pseudo-partial waves $\tilde{\phi}_i$ are equivalent to the AE partial waves outside a core radius r_c^l and match continuously onto ϕ_i inside the core radius. The core radius r_c^l is usually chosen approximately around half the nearest neighbour distance. The projector functions $\tilde{p}_i$ are dual to the partial waves:

$$\langle \tilde{p}_i|\tilde{\phi}_j\rangle = \delta_{ij}\,. \tag{9}$$

Starting from Eq. (7) it is possible to show that in the PAW method, the AE total density matrix is given by (for details we refer to Ref. [6]):

$$n^{\alpha\beta}(\mathbf{r}) = \tilde{n}^{\alpha\beta}(\mathbf{r}) + {}^1n^{\alpha\beta}(\mathbf{r}) - {}^1\tilde{n}^{\alpha\beta}(\mathbf{r}), \tag{10}$$

where $\tilde{n}$ is the soft pseudo-density matrix calculated directly from the pseudo-wavefunctions on a plane-wave grid (see Eq. (9) above and Eq. (15) of Ref. [6]) :

$$\tilde{n}^{\alpha\beta}(\mathbf{r}) = \sum_n f_n \langle \tilde{\Psi}_n^\beta|\mathbf{r}\rangle\langle\mathbf{r}|\tilde{\Psi}_n^\alpha\rangle. \tag{11}$$

The on-site density matrices ${}^1n$ and ${}^1\tilde{n}$ are treated on a radial support grid that extends up to r_{rad} around each ion. They are defined as (Eq. (16) and (17) of Ref. [6]):

$${}^1n^{\alpha\beta}(\mathbf{r}) = \sum_{(i,j)} \rho_{ij}^{\alpha\beta} \langle\phi_i|\mathbf{r}\rangle\langle\mathbf{r}|\phi_j\rangle, \tag{12}$$

$${}^1\tilde{n}^{\alpha\beta}(\mathbf{r}) = \sum_{(i,j)} \rho_{ij}^{\alpha\beta} \langle\tilde{\phi}_i|\mathbf{r}\rangle\langle\mathbf{r}|\tilde{\phi}_j\rangle. \tag{13}$$

$\rho_{ij}^{\alpha\beta}$ are the occupancies of each augmentation-channel (i,j) and they are calculated from the pseudo-wavefunctions applying the projector functions:

$$\rho_{ij}^{\alpha\beta} = \sum_n f_n \langle \tilde{\Psi}_n^\beta|\tilde{p}_i\rangle\langle\tilde{p}_j|\tilde{\Psi}_n^\alpha\rangle. \tag{14}$$

For a complete set of projectors the charge density ${}^1\tilde{n}$ is exactly the same as $\tilde{n}$ within the augmentation spheres. In the PAW approach, the pseudo-wavefunctions $\tilde{\Psi}_n^\alpha$ fulfil the following generalised orthogonality condition:

$$\sum_\alpha \langle \tilde{\Psi}_n^\alpha|S^{\alpha\alpha}|\tilde{\Psi}_m^\alpha\rangle = \delta_{nm}, \tag{15}$$

where the overlap operator is defined by:

$$S^{\alpha\beta}[\{\mathbf{R}\}] = \delta_{\alpha\beta}\left(1 + \sum_i |\tilde{p}_i\rangle q_{ij}\langle\tilde{p}_j|\right), \tag{16}$$

and q_{ij} is given by:

$$q_{ij} = \langle \phi_i | \phi_j \rangle - \langle \tilde{\phi}_i | \tilde{\phi}_j \rangle \tag{17}$$

The pseudo-wavefunctions are obtained by solving the generalised Kohn-Sham equations

$$\sum_{\beta} H^{\alpha\beta} | \tilde{\Psi}_n^{\beta} \rangle = \epsilon_n S^{\alpha\alpha} | \tilde{\Psi}_n^{\alpha} \rangle. \tag{18}$$

Forces are usually defined as the total derivative of the energy with respect to the ionic positions

$$\mathbf{F} = -\frac{d\,E}{d\mathbf{R}} \tag{19}$$

In the PAW method (as in the US-PP method), complications arise from the fact that the augmentation spheres and compensation densities are allowed to move with the ions, which gives rise to additional terms (similar to Pulay forces) in comparison with standard plane-wave codes. These correction terms are described in detail by Kresse and Joubert [7], the generalisation to noncollinear magnetisation densities is straightforward.

Applications: Small metallic clusters

Small clusters of Fe_n (n $\leq$ 5) have been studied extensively in the past and represent ideal systems for testing our implementation of noncollinear magnetism. As fcc Fe is known to have a spin-spiral ground-state, noncollinear magnetism is suggested to be important in Fe clusters, primarily as they have less symmetry constraints than bulk materials. The magnetic ground state of body-centred cubic chromium is a spin-density-wave state described as a long-period modulation ($\sim$ 20 interatomic distances) of a simple type-I antiferromagnetic structure [17], with a modest magnetic moment of $M_{Cr} \sim 0.6\ \mu_B$. However, there is evidence that in a case of

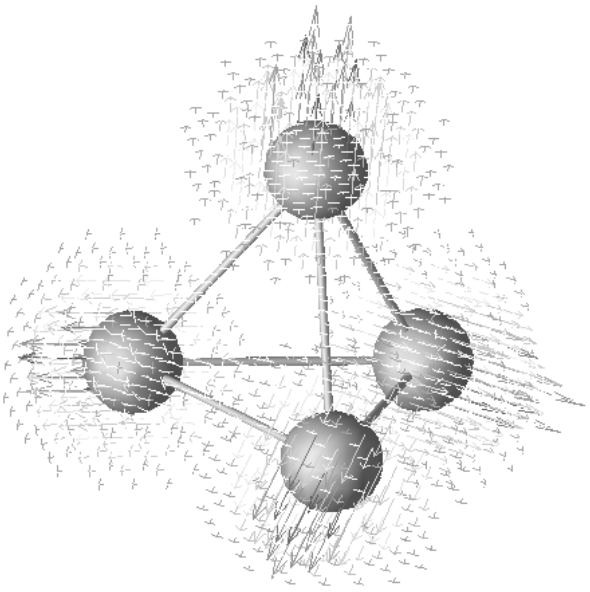

Figure 2: A three dimensional view of the magnetisation density surrounding Cr_4 atoms. The iso-surface plots indicate that the magnetisation density is spherically symmetric at all large density values. Only in the 'Bloch wall' region does the direction of magnetisation change, the magnetic vectors rotate in the 'Bloch wall' but also tend to zero in this region.

reduced coordination (e.g. at a surface) the Cr moment is strongly enhanced - $M_{Cr} \sim 2.5\ \mu_B$ has been reported [18, 19] for a Cr(100) surface. With this in mind we have investigated the likely ground-state configurations of small Cr_n ($n \leq 5$) clusters. We expect large magnetic moments and strong antiferromagnetic nearest neighbour coupling. In the triangular like configurations this will inevitably lead to frustration and hence possibly to noncollinear states.

Tetrahedral Cr_4 is rather interesting in terms of noncollinear arrangements of the magnetic moments. We found three solutions, a metastable FM one with small bulk-like moments, a noncollinear metastable state, which is the 3D generalisation of the 120° arrangements found in frustrated antiferromagnetic 2D lattices with the magnetisation directions on the neighbouring atoms forming a tetrahedral angle of $\sim 109.5°$, and an AFM ground-state. In both the AFM and noncollinear states large magnetic moments are predicted. The AFM ground-state is $\sim$ 160 meV/atom (GGA) lower in energy than the noncollinear configuration. The structure is distorted unlike the FM and noncollinear cases with very large distances of 2.97 Å between ferromagnetically coupled atoms and slightly shorter bonds in AFM pairs. The noncollinear solution has a bond-length of 2.58 Å in GGA which is intermediate between the long bonds in the AFM and the short bonds in the FM configurations. In the noncollinear case the total atomic magnetic moment is $\sim 4.02\ \mu_B$/atom in the GGA and is symmetric on all sites. Fig. 2 shows a plot of the magnetisation density for this solution. The magnetisation density varies smoothly with position and is localised symmetrically around the atomic sites as depicted in Fig. 2.

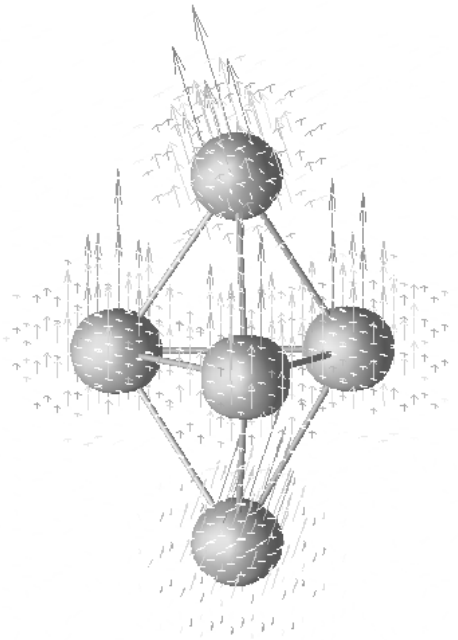

Figure 3: A three dimensional view of the magnetisation density surrounding Fe_5 atoms. The iso-surface plots indicate that the magnetisation density is spherically symmetric at all large density values on the apical atoms only, but is slightly 'squashed' at the central atomic sites. Only in the 'Bloch wall' region does the direction of magnetisation change, the magnetic vectors rotate in the 'Bloch wall' but also tend to zero in this region.

A case of particular interest in the work of Oda *et al.* [1] is the Fe_5 bipyramidal structure in which they found the roughly FM ground-state to contain tilted magnetic moments on the apical atoms of the bipyramid. Intuitively such solutions seem to be unphysical as they break the normal collinear symmetry and one would expect the total energy to be higher.

For the Fe_5 bipyramidal cluster our calculations have been able to stabilise a noncollinear solution some $\sim$ 14 meV/atom below the collinear results. In the noncollinear ground-state as well as in the metastable collinear ferromagnetic state, the bond-lengths in the central triangle are slightly longer than between the central and the apical atoms. This somewhat squashed but otherwise undistorted structure agrees with the results of Oda *et al.* [1], but disagrees with the work of Castro and Salahub [20]. The tilt angle of the magnetic moment is $\sim$31.3° in GGA, to be compared to $\sim$29.7° in the LDA calculation of Oda *et al.* How such frustration might arise is not immediately clear. Certainly, the coupling between the apical atoms must play a crucial role in establishing the frustration. As the moments on the apical atoms tilt in opposite directions, it appears that the exchange interactions between the apical atoms is antiferromagnetic and hence acts against the ferromagnetic nearest neighbour coupling between apical and central atoms. Hence a rotation of the apical moments relative to those in the central triangle allows the magnetic energy to be optimised. A detailed analysis of the exchange coupling would be valuable to obtain better understanding of the conditions responsible for the frustration. Finally, Fig. 3 shows the magnetisation density surrounding the atomic sites. The figure illustrates, firstly, that the magnetisation density varies smoothly with position, secondly, that the spin-direction only changes at the 'Bloch wall' between atoms where the charge- and spin-densities are small and thirdly that the magnetisation density is roughly uniform in the magnetic region of the atoms. However, one can just see that for the central atoms the magnetisation density deviates from being spherically symmetric and exhibits a somewhat 'squashed' appearance.

Applications: Cr and Mn overlayers on the Cu(111) substrate

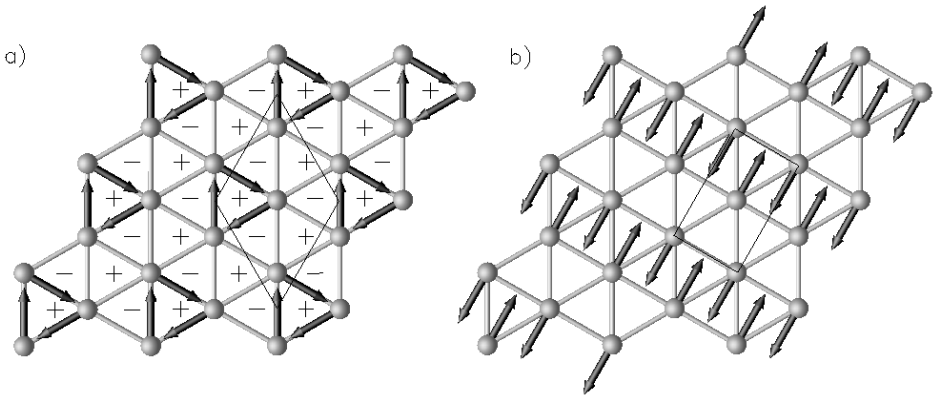

Figure 4: (a) Noncollinear magnetic structure of triangular layers corresponding to the frustrated XY-models with nearest-neighbour interactions. The relative directions of the magnetic moments (neglecting spin-orbit coupling) are indicated by the arrows. + and − signs indicate the helicities assigned to the elementary triangles (cf. text). The primitive $(\sqrt{3} \times \sqrt{3})$ unit cell is indicated by the thin lines. (b) Row-wise antiferromagnetic structure of triangular layers. Arrows indicate the relative directions of the magnetic moments, the thin lines show the c(2×2) unit cell.

One of the simplest examples of a frustrated two-dimensional spin system, where no perfectly collinear magnetic arrangement can be accommodated, is the antiferromagnetic planar (XY) model with nearest-neighbour interactions on a triangular lattice. Antiferromagnetic interactions

are a source of magnetic frustration on the triangular lattice. The ground states of such systems tend to consist of spins ordered on three interpenetrating sublattices with lattice vectors of length $\sqrt{3}a$ while spins on different sublattices are orientated $\pm 120°$ to each other (see Fig. 4). Wannier [21] proved that by considering the ground state energy of any single elementary triangle and minimising the energy with respect to two of the spin angles one obtains ground states for the triangle in which the spins form $\pm 120°$.

Freestanding triangular Cr and Mn monolayers

Fig. 5 summarises our results for the magnetic moments and total energies of the three possible magnetic configurations as a function of the nearest-neighbour bond-length. In both Cr and Mn monolayers, a ferromagnetic high-spin phase with a magnetic moment of nearly 4 μ_B is stable only at expanded interatomic distances. In Cr monolayers the magnetic moment breaks down rather suddenly at a bond-length of about 2.57 Å, the ferromagnetic minimum being about 280 meV higher in energy than the non-magnetic minimum. In Mn monolayers we find a transition from a ferromagnetic high-spin phase at bond-lengths larger than 2.47 Å to a ferromagnetic low-spin phase at closer interatomic distances. The low-spin phase (M $\leq$ 1.5 μ_B) looses its magnetic moment only at strongly reduced bond-lengths.

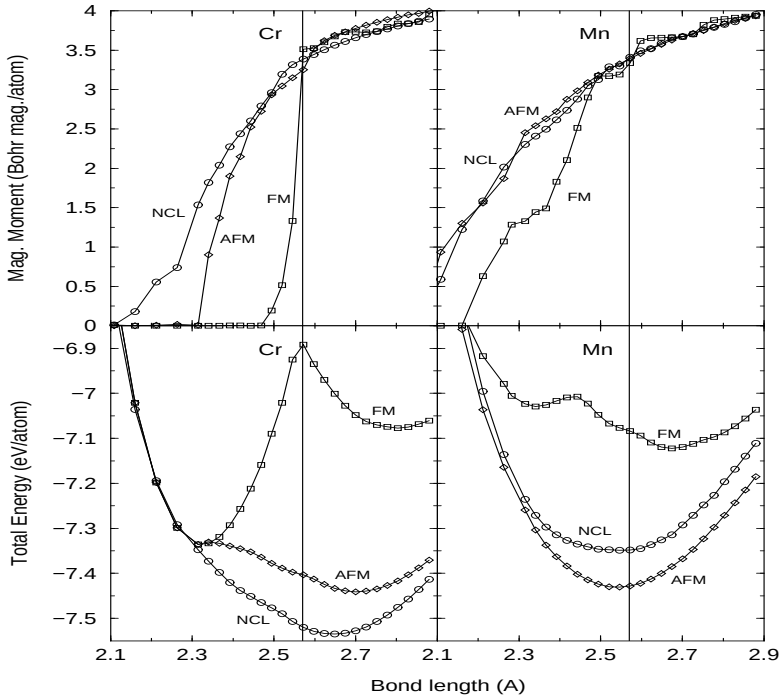

Figure 5: Total energy and magnetic moments of the ferromagnetic $p(1\times1)$, the antiferromagnetic $c(2\times2)$, and the noncollinear ($\sqrt{3}\times\sqrt{3}$) phases of freestanding triangular Cr and Mn monolayers as a function of the nearest neighbour bond-length. The vertical lines mark the lateral interatomic distance of a Cu(111) substrate.

The row-wise antiferromagnetic $c(2\times2)$ Cr monolayer has an equilibrium bond-length of 2.70 Å at a magnetic moment of 3.75 μ_B. Under compression the magnetic moment is strongly reduced, it disappears at a bond-length of 2.31 Å corresponding roughly to the bond-length of the nonmagnetic phase. The noncollinear 120° phase represents the magnetic ground state, the equilibrium bond-length is about 2.65 Å, at these distances, the magnetic moment is slightly smaller

than in the antiferromagnetic phase. Under compression, the noncollinear magnetic moments are gradually reduced. They disappear at distances somewhat smaller than the equilibrium distances in the nonmagnetic phase.

In Mn monolayers the relative stability of the antiferromagnetic and noncollinear phase is reversed (see Fig 5), the equilibrium bond-lengths and magnetic moments being almost the same in both phases. Under compression the magnetic energy difference is quickly reduced, at bond-lengths smaller than about 2.35 Å, both phases are energetically almost degenerate. The antiferromagnetic ground-state in Mn is somewhat surprising, to investigate this point further we now consider triangular Cr and Mn overlayers on Cu(111).

Triangular Cr and Mn overlayers on Cu(111)

For overlayers adsorbed on Cu(111) substrates the same three magnetic configurations have been considered. For comparison, the vertical lines in Fig. 5 show the lateral lattice constant of the Cu(111) substrate. We find that triangular Mn-layers show an almost ideal epitaxial match to the substrate, whereas adsorbed Cr-layers undergo a small compressive strain. In both the antiferromagnetic and the noncollinear phases, the magnetic moments are reduced compared to the freestanding monolayer. The important point is that for Mn/Cu(111) the antiferromagnetic phase remains energetically favoured.

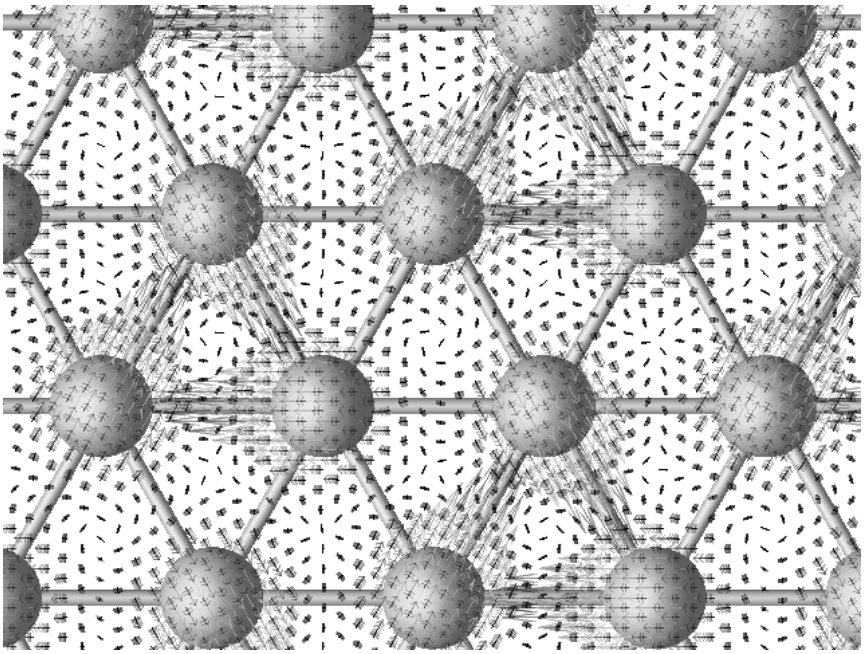

Figure 6: Vector field of the magnetisation density for the noncollinear phase of Cr on Cu(111). The relative direction of the magnetisation density (neglecting spin-orbit coupling) is indicated by the arrows, the length of each arrow is proportional to the absolute value of the local magnetisation density.

The different behaviour of triangular layers of Cr and Mn is clearly related to the rather long-range nature of the exchange interactions in the Mn layers, as already pointed out by Spišák and Hafner [22]. In the noncollinear phase, first and third neighbours carry magnetic moments with a relative 120° orientation, but second neighbour-moments are ferromagnetically aligned (see Fig. 4). In the row-wise antiferromagnetic structure out of six nearest and next-

nearest-neighbour atoms four are aligned antiferromagnetically and two ferromagnetically in each shell. All six sites in the third-neighbour shell show ferromagnetic alignment. If the exchange-interaction is antiferromagnetic for the first two shells and ferromagnetic for the third shell, the frustration may be weaker in the collinear phase.

Fig. 6 shows the magnetisation density calculated for the noncollinear phase of Cr on Cu(111). The local direction of the magnetic moment is indicated by the arrows, the length of the arrows being proportional to the absolute value of the magnetisation density. In addition, around each site iso-surfaces of the magnetisation densities are drawn. At a first look one tends to conclude that the magnetisation densities are fairly well localised and as the iso-surfaces are also almost spherical at reasonably large values, the conclusion that the AMA is a reasonable choice in this system seems to be appropriate. However, the regions around the atoms in which the direction of magnetisation is approximately constant are distinctly smaller than the muffin-tin spheres of the FLAPW method or the overlapping atomic spheres of the LMTO approach. Interesting new aspects of this study are seen precisely in the bonding and interstitial regions where the direction of the magnetisation changes.

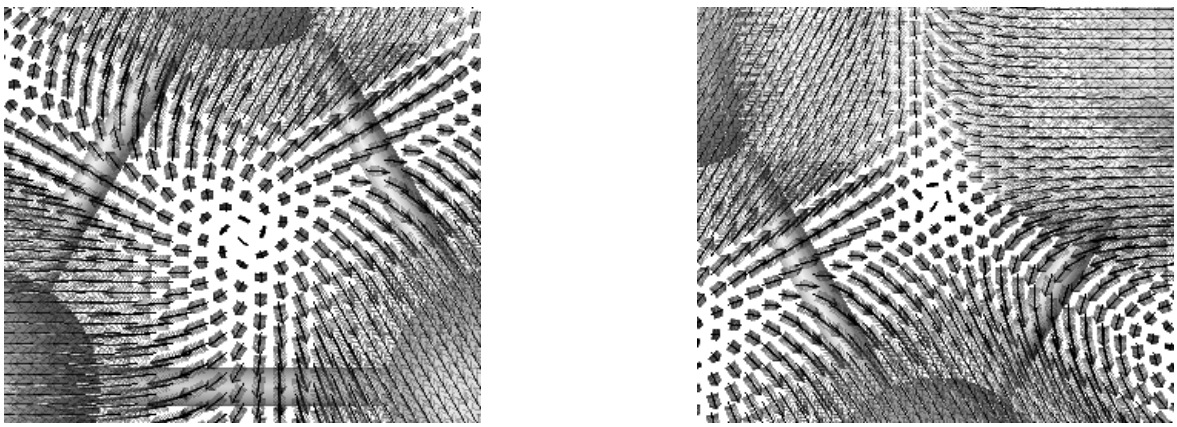

Figure 7: Enlarged view of an outward spiral-vortex and an anti-vortex. Cf. text.

In Figs. 7 and 8 we recognise characteristic patterns in the vector field of the magnetisation density: Inside the elementary triangles to which a positive helicity has been assigned, the vector field forms a vortex which may be a clockwise or a counterclockwise spiral or show a circular pattern, inside the triangles with negative helicity we find anti-vortex patterns related to each other by 120° rotations. Detailed views of the three types of vortices are show in Figs. 7 and 8. Spiral vortices are formed inside the triangles where the direction of the magnetisation is aligned (for the given alignment of the magnetisation directions with respect to the crystal lattice) along the bond directions, pointing either away from or into the triangle. In both cases the direction of magnetisation in the bond centres is perpendicular to the bonds, in the former case the vectors point out of the triangle and an outward spiral is formed, in the latter case the vectors point towards the centre of the triangle such that an inward spiral is formed. A circular vortex is formed within those triangles where the magnetisation at the lattice sites is perpendicular to one of the edges of the triangle. In the bond centres, the magnetisation is in this case aligned along the bond directions. An example for an anti-vortex structure realized in triangles with negative helicity is shown on the right side of Fig. 7. In this case the direction of magnetisation is perpendicular to two of the bonds (pointing either out of or into the triangle) and parallel

to the third bond. To the three different types of vortices correspond anti-vortex structures rotated by 120°. This picture also illustrates an important difference between the muffin-tin-like

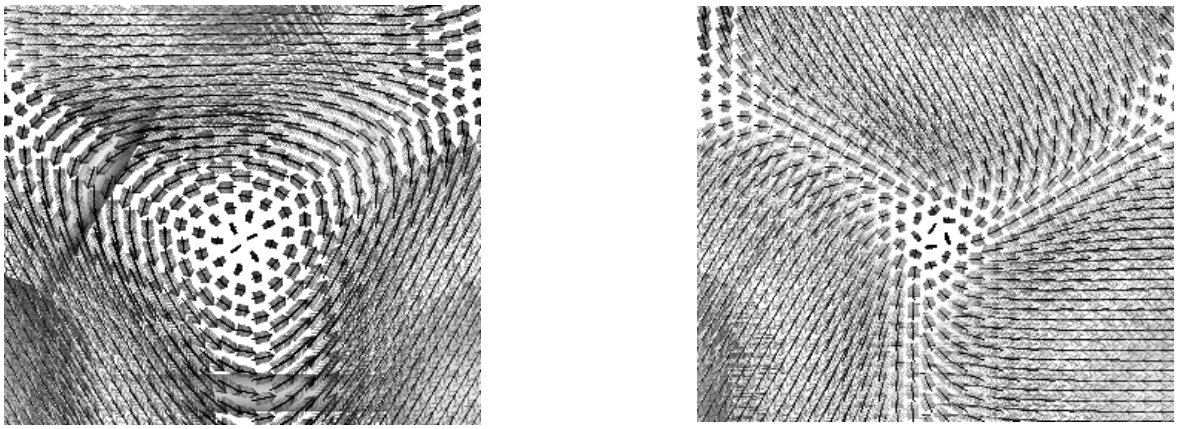

Figure 8: Enlarged view of a circular vortex and an inward spiral-vortex. Cf. text.

description of the magnetisation density within the FLAPW approach used by Asada *et al.* [4] and Kurz *et al.* [5] and the present PAW description. In the FLAPW-approach, the direction of magnetisation changes discontinuously at the muffin tin sphere boundaries. In the PAW description, the direction of magnetisation changes continuously and is (for the present choice of the global alignment) at these points either parallel or perpendicular to the bond, depending on its local environment. It is also interesting to point out that the bond-centres form a Kagomé lattice dual to the triangular lattice of the atoms. The six triangles surrounding a hexagon of the Kagomé lattice contain an alternating anti-vortex or vortex, the existence of three different types leading to further symmetry breaking analogous to the positive and negative helicities. This point certainly deserves further investigation.

Expected Impact

The approach described above has clearly been developed with the intention of studying problems in which magnetisation density is not well localised on atomic sites, in addition to more conventional cases. Examples of such weak localisation, for which the atomic moment approximation is more questionable, occur in materials such as disordered magnetic intermetallic compounds, amorphous alloys and structures with antiferromagnetically coupled atoms on sublattices necessarily leading to frustration (e.g. triangular layers and Kagomé lattices). As advancing computer technology allows us to explore more complex atomic structures such an approach will hopefully prove invaluable.

Acknowledgements

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