Ψ_k Newsletter

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

Number 33 June 1999

Editor: Z. (Dzidka) Szotek
E-mail: psik-coord@daresbury.ac.uk

Contents

1 Editorial

In the section **News from the TMR1 Network** readers will find a report on the annual meeting and midterm review of the **TMR1** network that took place in Aussois. It contains also the programme and about 50 abstracts. In the same section we also have a report on 'Hands-on Dichroism Course', and a postdoc position announcement. In the **ESF** section readers will find a report with the programme and abstracts of the 'Workshop on Hydrogen in Semiconductors'. In this section there is also a report on a collaborative visit of C. Filippi to Berlin. In the **TMR2** network sections there is a TMR position announcement from Würzburg. Also, in the general sections advertising positions and forthcoming workshops/conferences readers will find a few interesting announcements. As always, we have a number of abstracts in the usual **Abstracts** section. The scientific highlight is by Balazs Gyorffy (Bristol) *et al.* on **'Quasi-particles and Van Hove Scenario for the Superconducting Cuprates'**. Please check the table of content for further details.

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

http://www.dl.ac.uk/TCSC/HCM/PSIK/main.html

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@daresbury.ac.uk

2 General News

2.1 Psi-k2000 Conference

Schwäbisch Gmünd, 22-26 August, 2000

”Ab initio (from Electronic Structure) Calculations of Complex Processes in Materials

This is just to inform you that additionally to the web address

`http://www.dl.ac.uk/TCSC/HCM/PSIK/Psi-k2000.html`,

the information on the Psi-k2000 Conference can also be reached from the web page of the Computational Science and Engineering Department of the Daresbury Laboratory, UK at:

`http://www.cse.clrc.ac.uk/Activity/Psi-k2000`.

The poster announcing the conference has been designed and is soon to be distributed to the universities and key research institutions around the world.

Please keep on checking for an updated information on the **Psi-k 2000 Conference**.

3 News from the TMR1 Network

”Ab Initio Calculations of Magnetic Properties of Surfaces, Interfaces and Multilayers”

3.1 Reports on Workshops

3.1.1 Report on the Annual Meeting in Aussois

Third Annual Meeting: ’Interface Magnetism’

Aussois, March 28-31, 1999

This annual meeting was associated with a midterm review conducted by an EU official, Dr. Gerburg Larsen, and an EU appointed expert, Professor Jakob Bohr. The meeting was attended by 84 people, representing all partners of the TMR network on ’Interface Magnetism’. All TMR postdocs and Ph. D. students, and other young researchers delivered short talks both at the meeting and during the one-day review by Brussels, which took place on Tuesday, March 30. The agenda and programme of the midterm review is not included in the attached scientific programme of the annual meeting.

As can be seen from the programme of the meeting, the longer talks were by senior members of the Network, usually giving a broad introduction to the variety of flagship projects of the network. The attached abstracts of the presented talks give a broad overview of the state of the projects undertaken by the network. Most of the talks were concerned with applications, but there were also some concerned with developments of large computer codes and their first applications to real problems.

Both the meeting and the midterm review were very successful, giving us confidence in the work done by all the partners of the network. Especially, the impact that our research has worldwide is very motivating to the young researchers employed by the network.

This was already the third annual meeting of this TMR network. These annual meetings of the network have seen a steady increase in the number of participants from about 60 to over 80, reflecting the growth of its scientific activities. Next year’s annual meeting will take place during the Psi-k2000 Conference in Schwäbisch Gmünd, on August 22-26. At the conference this TMR network will be responsible for organising several symposia.

The programme of the meeting follows.

Sunday 28 March 1999

9:00 9:30	Peter Weinberger (Vienna) **Perpendicular Magnetism in CoPt superstructures on Pt substrates**
9:30-9:45	Peter James (Uppsala) **Magnetic anisotropy ...**
9:45-10:00	Christoph Uiberacker (Vienna) **Perpendicular magnetism in the system Cu(100)/Ni$_n$ and Cu(100)/Ni$_n$/Co$_m$**
10:00-10:15	M. Eisenbach (Bristol) **Magnetic States on an inhomogeneous wire**
10:15-10:30	Erik Holmstrom (Uppsala) **Interlayer exchange coupling in Fe/Pd**
10:30-11:00	Coffee
11:00-11:15	J. Opitz (Dresden) **Interlayer-exchange coupling in Fe/Au-multilayers**
11:15-11:30	F. Erler (Dresden) **GMR in finite layered Co/Cu-systems**
11:30-11:45	J. Binder (Dresden) **Anisotropic relaxation times of 3d impurities in Co/Cu-multilayers**
11:45-12:00	L. Sandratskii (Darmstadt) **Non-collinearity of magnetic structure in systems with low symmetry**
12:00-12:15	Ph. Kurz (Juelich) **Non-Collinear Magnetism of Magnetic Monolayers on Ag(111) and Cu(111)**
12:15-12:30	P.Mohn (Vienna) **Non-collinear magnetic states in the GMR system (Sr,Y)MnO3**
12:30	Lunch
17:00-17:30	R. Zeller (Juelich) **Parallel Computing with the KKR Method**
17:45-18:00	A. Settels (Juelich)**Different Methods for Lattice Relaxations within the KKR Formalism**
18:00-18:15	T. Korhonen (Juelich) **Effect of Lattice Relaxations on the Hyperfine Fields of Heavy Impurities in Fe**
18:15-18:30	B. Nonas (Juelich) **Relativistic Ab-Initio Calculations for Impurities on Surfaces**
18:30-19:00	Coffee
19:00-19:15	V. Bellini (Juelich) **A TB-KKR Study of Magnetic Moments and Hyperfine Fields at the Fe/Co Interface**
19:15-19:30	Ch. Zecha (Muenchen) **A new method to deal with large lattice distortions within the KKR-formalism**
19:30-19:45	L. Petit (Daresbury) **Screened real-space study of the magnetic properties of the transition metals**
19:45-20:00	R. Abt (Juelich) **Magnetism, Structure and Alloy Formation of Ultrathin Films**
20:00	Dinner

Monday 29 March 1999

9:00-9:30	P. Bruno (Halle) **Theoretical approaches of spin-electronics**
9:30-9:45	C. Blaas (Vienna) **Resistivities and GMR for the MOTOROLA spinvalve**
9:45-10:00	P. Zahn (Dresden) **Spin polarization in magnetic tunnel junctions**
10:00-10:15	N. N. Lathiotakis (Bristol) **Asymptotic behaviour of the Oscillatory Exchange Coupling in Magnetic Multilayers**
10:15-10:30	A. Brataas (Delft) **Domain wall resistance in ferromagnets**
10:30-11:00	Coffee
11:00-11:30	J. Schwitalla (Bristol) **On the first-principles approach to the theory of Bloch Walls**
11:30-12:00	W. Hofer (Vienna) **STM: Simulation of the tunnel current from first principles electronic structure calculations: magnetic surfaces**
12:00-12:15	S. Bluegel (Juelich) **Magnetic Surfaces under Static External Electric Fields**
12:15-12:30	N. Papanikolaou (Juelich) **STM-Spectra for Transition Metal Impurities on the Fe(001) Surface**
12:30	Lunch
17:00-17:30	G. Van der Laan (Daresbury) **X-ray magnetic dichroism shows every atom has its moments**
17:30-17:45	V. Popescu (Muenchen) **A fully relativistic theory of magnetic EXAFS**
17:45-18:00	I. Galanakis (Strasbourg) **Theoretical x-ray magnetic circular dichroism study of the magnetic properties of Fe ultrathin films on W(110) and of Co(50)Pt(50) thin films**
18:00-18:15	U Pustogowa (Vienna) **Is spin-resolved Auger spectroscopy a possible tool for magnetic domain mapping?**
18:15-18:30	J. Henk (Uppsala) **Magnetic structure and anisotropy of ultra-thin Ni films on Cu(001)**
18:30-19:00	Coffee
19:00-19:15	K. Xia (Eindhoven) **Calculating interface reflection and transmission matrices from first-principles using localized-orbital bases**
19:15-19:30	Lars Nordstrom (Uppsala) **Spin density waves in Cr films**
19:30-19:45	A.Ernst (Daresbury) **Photoemission calculations of 3d-metal surfaces and multilayers**
19:45-20:00	L. Szunyogh (Vienna) **Fully relativistic spin-polarized calculations of magneto-optical properties in thin Co/Pt films**
20:00	Dinner

Wednesday 31 March 1999

9:00-9:30	I. Abrikosov(Uppsala) **Understanding of Invar effect in Fe-Ni alloys**
9:30-9:45	M. Freyss (Strasbourg) **Interfacial alloying: influence of the chemical order on magnetic order**
9:45-10:00	J. Minar (Muenchen) **A fully relativistic theory for spin-polarized Auger spectroscopy**
10:00-10:45	T. Huhne (Muenchen) **Calculation of magneto-optical properties of layered systems by means of the SPR-KKR-method**
10:15-10:30	A. Vernes (Muenchen) **Galvano-magnetic properties of the alloy systems Cu-Ni and Cr-Ni**
10:30-11:00	Coffee
11:00-11:15	E. Arola (Bath) **Relativistic scattering theory of magnetisation-induced second harmonic generation**
11:15-11:30	S. Ostanin (Strasbourg) **Calculation of magnetic X-ray emission dichroism in disordered Co-Rh-based ternary alloys**
11:30-11:45	H. Freyer (Muenchen) **Fully relativistic calculations of the spin- and orbital susceptibility and Knight-shift in homogeneous and non-homogeneous systems**
11:45-12:00	M. Woods (Keele) **Relativistic Theory of Photoemission from Magnetic Surfaces**
12:00	Lunch
18:00-18:15	J. Izquierdo (Valladolid) **Magnetic properties of supported transistion-metal nanostructure**
18:15-18:30	M. Deng (Muenchen) **Magnetic properties of 5d-impurities in bcc-Fe**
18:30-18:45	S A Razee (Warwick) **”Local moments” and the electronic structure of ultra-thin Fe fims above their Curie temperatures**
18:45-19:00	L. Pourovskii (Uppsala) **Magnetic properties and surface energy of Ni monolayer on Cu substrate**
19:00-19:15	V. Crisan (Muenchen) **Electronic properties of the ternary systems Cu-Zn-Al**
19:15-19:30	Pavel Korzhavyi (Uppsala) **The effect of magnetism on the vacancy formation energy in 3d metals**
20:00	Dinner

Magnetic properties of thin films of Co and of (CoPt) superstructures on Pt(100) and Pt(111)

U. Pustogowa[1], J. Zabloudil[1],
C. Uiberacker[2], C. Blaas[2], P. Weinberger[2]
L. Szunyogh[1,3], and C. B. Sommers[4]

[1] *Center for Computational Materials Science, Vienna, Austria*
[2]*Institut für Technische Elektrochemie und Festkörperchemie,*
Technische Universität Wien, Vienna, Austria
[3] *Department of Theoretical Physics, Technical University Budapest,Budapest, Hungary*
[4]*Laboratoire de Physique des Solides, Université de Paris-Sud,Orsay, France*

Abstract

The magnetic properties of $\mathrm{Co}_n/\mathrm{Pt}(100)$, $\mathrm{Co}_n/\mathrm{Pt}(111)$, $(\mathrm{Co}_{0.5}\mathrm{Pt}_{0.5})_n/\mathrm{Pt}(100)$, $(\mathrm{CoPt})_n/\mathrm{Pt}(100)$ and $(\mathrm{CoPt})_n/\mathrm{Pt}(111)$, $n \leq 15$, are investigated using the fully relativistic spin-polarized Screened Korringa-Kohn-Rostoker method. It is found that only the artificial superstructures $(\mathrm{CoPt})_n/\mathrm{Pt}(100)$ and $(\mathrm{CoPt})_n/\mathrm{Pt}(111)$ show a perpendicular magnetic anisotropy beyond $n = 10$. For the free surfaces of Co on Pt in the case of the (100) orientation a multiple reorientation transition below $n = 7$ is found, while along (111) such a transition is predicted at about 4 layers of Co. For the homogeneous, statistically disordered alloy $\mathrm{Co}_{0.5}\mathrm{Pt}_{0.5}$ on Pt(100) the orientation of the magnetization remains in-plane for all n investigated. A comparison to experiment yields an interesting insight into aspects of order and disorder, surface segregation and phase separation frequently encountered in experimental studies of perpendicular magnetism in the Co/Pt system.

Perpendicular magnetism in the system $\mathrm{Cu}(100)/\mathrm{Ni}_n$ and $\mathrm{Cu}(100)/\mathrm{Ni}_n/\mathrm{Co}_m$

C. Uiberacker, J. Zabloudil and P. Weinberger
Institut für Technische Elektrochemie and Center of Computational Materials Science
Technical University Vienna, Getreidemarkt 9/158, A-1060 Wien, Austria
L. Szunyogh
Department of Theoretical Physics, Technical University Budapest
Budafoki út. 8, H-1521 Budapest, Hungary
and
Center of Computational Materials Science, Technical University Vienna
Getreidemarkt 9/158, A-1060 Wien, Austria
C. Sommers
Laboratoire de Physique des Solides, Bat. 510,
Campus d'Orsay, 91405 Orsay, France

Abstract

The magnetic anisotropy energy of $\mathrm{Ni}_n/\mathrm{Cu}(100)$ and $\mathrm{Co}_n/\mathrm{Ni}_n/\mathrm{Cu}(100)$ is calculated in terms of the spin-polarized fully relativistic Korringa-Kohn-Rostoker method including

surface relaxation by using 2D structure constants originally described for LEED calculations. Investigating different numbers of relaxed Ni-layers, the reorientation transition of Cu(100)/Ni$_n$ back from perpendicular to in-plane can be compared to the experiment. The reorientation occurs due to the dipole-dipole energy of the unrelaxed Ni layers. Furthermore, by putting a fixed number of Co-layers on top, the reorientation transition occurs earlier due to the bigger moment and respectively bigger dipole-dipole energy of the Co-layers.

States of orientation along a magnetically inhomogeneous nano wire

M. Eisenbach, B. L. Györffy

Abstract

We investigate the magnetic states of nano wires (diameter 50 − 500 Å) which consist of disc shaped magnetic segments separetad by non-magnetic spacers. To descibe this system we propose a simple classical one dimensional spin model and study its consequences. In particular we examine the ground state and thermal behaviour as function of both anisotropy of the ferromagnetic discs and thickness of the non magnetic spacer. We find a rich structure of possible ground states and a temperature driven reorientations of the magnetic moments in various regions of the parameter space.

We shall also report on our preliminary investigation of the above system in terms of an itenerant model based on mobile electrons and their spins. The Hubbard like model investigated here incooperates the dipolar interaction between the magnetic moments at different sites, and we are able to calculate the shape anisotropy of a disc in the Hartee-Fock approximation of our itinerant model.

Magnetic Interlayer Coupling in Fe/Pd Multilayers

E. Holmström, A. Niklasson, L. Nordström, I. Abrikosov and
B. Johansson

Condensed Matter Theory Group, Department of Physics, Uppsala University, Box 530, 751 21 Uppsala, Sweden

Abstract

Magnetic properties of Fe/Pd (100) multilayers have been calculated using a first principles TB-LMTO Green's function method. We investigate how the magnetic interlayer coupling is changed when the magnetic moment of the Fe layers is suppressed. A complex non-RKKY like behaviour of the interlayer coupling as function of Fe magnetic moment was found, indicating the influence of magnetic enhancement effects in Pd. An oscillatory behaviour of the induced Pd moment as function of Pd spacer thickness is found and explained in terms of quantum confinement.

Interlayer Exchange Coupling in Fe/Au-Multilayers

J. Opitz, P. Zahn and I. Mertig

TU Dresden, Institut für Theoretische Physik, D-01062 Dresden, Germany

Abstract

The coupling strength of the Interlayer Exchange Coupling (IEC) in magnetic multilayer systems is strongly determined by the quality of the interfaces between magnetic and non-magnetic layers. Consequently, theoretical and experimental results differ in general by an order of magnitude. New measurements for Fe/Au samples of high structural quality have been performed recently [1]. The obtained coupling strength ($J \approx 1mJ/m^2$) is much higher than for other multilayer sytems. The aim of this paper is to present ab initio calculations for Fe/Au (001) multilayers with the same sample dimensions as in the experiments. The structure is characterized by an fcc-bcc-transition. The calculations are based on density functional theory using a scalar-relativistic Screened KKR method. Ideal interfaces between Fe and Au are assumed. IEC is obtained by the comparison of the single particle energies for parallel and antiparallel magnetic configuration of the multilayer (Frozen Potential Approximation).

[1] J. Unguris, R.J. Celotta, and D.T. Pierce, Phys. Rev.Lett. 79, 2734 (1997).

GMR in finite layered Co/Cu-systems

F. Erler, P. Zahn and I. Mertig

TU Dresden, Institut für Theoretische Physik, D-01062 Dresden,Germany

Abstract

Ab initio calculations for Current-In-Plane Giant MagnetoResistance (CIP-GMR) of finite Co/Cu (100)-multilayers are presented. The influence of the finite size of the sample and of the number of Co/Cu-bilayers, that is, Co/Cu-interfaces in the sample is discussed. The calculations are based on density functional theory using a Screened KKR method. Since the method is N-scaling unit cells with up to 500 Atoms can be treated. The in-plane conductivity of the sample with parallel and antiparallel orientation of the magnetic moments is calculated by solving the Boltzmann equation in relaxation time approximation.
In agreement with experiments [1] the GMR ratios increase linearly with the number of bilayers for small numbers and saturate for larger numbers.

[1] L. v. Loyen and C. M. Schneider, private communication.

Anisotropic relaxation times of 3d impurities in Co/Cu-multilayers

J. Binder, P. Zahn and I. Mertig

TU Dresden, Institut für Theoretische Physik, D-01062 Dresden,Germany

Abstract

Spin-dependent scattering is considered to be the origin of Giant MagnetoResistance (GMR) in magnetic multilayers, although the role of bulk or interface defects is still under discussion.

We present the first ab initio calculations for anisotropic relaxation times of 3d impurities as a function of the impurity position in a Co/Cu-multilayer. The calculations are performed within spin density functional theory using a Green function method (Screened Korringa-Kohn-Rostoker method). The impurity potential was calculated selfconsistently solving a Dyson equation.

It will be shown that the local densities of states, the local moments and especially the spin anisotropy of scattering depend strongly on the impurity position.

Non-collinearity of magnetic structure in systems with low symmetry

L.M. Sandratskii

Institut für Festkörperphysik, Technische Universität, D-64289 Darmstadt, Germany

Abstract

In our recent publications [1] (see also [2] for review) we have shown that in relativistic systems with low symmetry the magnetic structure must be noncollinear. Here, the application of these principles to the multilayer systems is discussed.

1. L.M. Sandratskii, J. Kübler, PRL 75 (1995) 946; Physica B, 217 (1996) 167; Europhysics Letters, 33 (1996) 447; PRL 76 (1996) 4963; PRB 55 (1997) 11395.

2. L.M. Sandratskii, Advances in Physics 47 (1998) 91.

Non-Collinear Magnetism of Magnetic Monolayers on Ag(111) and Cu(111)

Philipp Kurz, Gustav Bihlmayer and Stefan Blügel

Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich,

Abstract

We discuss the magnetic structure of Cr and Mn monolayers on Cu(111) and Ag(111) surfaces. The nearest neighbor interaction of Cr and Mn is antiferromagnetic. Assuming a Heisenberg model for the description of these monolayer systems on the triangular lattice of the (111) substrate, we expect a non-collinear spin structure as ground state for these monolayers with a magnetic moment which is rotated to the moments of the neighboring atoms by $\pm 120^0$ [$(\sqrt{3} \times \sqrt{3})R30^o$ non-collinear spin structure]. We implemented the noncollinear magnetism on the basis of the vector-spin-density approach in the interstitial region into our film and bulk-FLAPW code and calculated the total energy as function of the angle between neighboring spins in the $(\sqrt{3} \times \sqrt{3})R30^o$ unit cell. While Cr behaves as expected surprises are found for Mn and the consequences for the MnCu/Cu(111) surface alloys are discussed. We investigate the stability of these systems against clustering and interdiffusion and compare with results for other surfaces: the interplay between alloy- and spin structure for various compositions leads to the stabilization of antiferromagnetic chains of Mn on this surface.

Non-Collinear Magnetic States in the GMR System (Y,Sr)MnO_3

P. Mohn and S. F. Matar*
Center for Computational Materials Science and Institut für Technische Elektrochemie und Festkörperchemie,
Technische Universität Wien, Vienna, Austria
**Institut de Chimie de la Matière Condensée de Bordeaux ICMCB-CNRS, Pessac, France*

Abstract

The perovskite system $(La_{1-x}Sr_x)MnO_3$ shows an antiferromagnetic insulating phase for $x = 0$ and changes to metallic ferromagnetism for $0.2 \leq x \leq 0.5$. At the phase boundaries where the AF and the FM phase are in energetic competition GMR behaviour has been found. Employing the Augmented Spherical Wave (ASW) method we investigate the isoelectronic system $(Y_{1-x}Sr_x)MnO_3$ on the basis of the virtual crystal approximation. As a function of x we find a rich variation of different magnetic states. In addition we study the formation of competing spin-canting states as suggested in [1].
[1] J. Inoue and S. Meakawa, Phys. Rev. Lett. **74** (1995) 3407.

Parallel Computing with the KKR Method

R. Zeller

Institut für Festkörperforschung, Forschungszentrum Jülich GmbH

Abstract

Because of the clear separation into single-site and multiple scattering properties the Korringa-Kohn-Rostoker method is very well suited for massively parallel large-scale electronic-structure calculations. One strategy is to distribute the calculation of the single-scattering quantities like t matrices and wave-functions to the computing nodes. This is trivial and must be combined with non-trivial distributed matrix inversions to obtain the multiple-scattering contributions. Fortunately, for these inversions efficient standard software packages (ScaLapack) exist. Another strategy is to distribute the mesh points for the energy integration which is used to obtain the electronic density. Both strategies have been implemented into our KKR codes and their advantages and disadvantages will be discussed. It will also be shown that both strategies can be used simultaneously.

Different Methods for Lattice Relaxations within the KKR-Formalism

A. Settels, T. Korhonen, R. Zeller, and P.H. Dederichs

Institut für Festkörperforschung, Forschungszentrum Jülich GmbH

Ch. Zecha, and H. Ebert

Institut für Physikalische Chemie, LMU München

Abstract

To calculate the electronic structure of defects in metals and semiconductors, it is very important to take lattice relaxations into account. In the KKR-formalism for lattice relaxations the host Greenfunction for the relaxed positions is constructed by a so called U-transformation. Due to the $l_{\max}$ cut-off this procedure leads for larger displacements to systematic errors since the coupling with higher angular momenta is neglected. By a change of the reference system in the Dyson-equation it is possible to separate the U-transformation from the time-consuming selfconsistency procedure. As a consequence the relaxations can be calculated with higher accuracy and less computing time. On the other hand it is possible to calculate the Greenfunction directly via a Brillouinzone-integration by introducing virtual basis atoms in the ideal host lattice. The latter method gives an exact Greenfunction for arbitrary positions. The different methods are compared and numerical advantages or disadvantages are discussed.

Effect of Lattice Relaxations on the Hyperfine Fields of Heavy Impurities in Fe

T. Korhonen, A. Settels, N. Papanikolaou, R. Zeller and P.H. Dederichs

Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich,

Abstract

We present first-principles calculations of hyperfine fields of heavy impurities in bcc Fe. In particular, the effect of lattice relaxations on the calculated hyperfine fields are studied. The calculations are based on a full-potential Korringa-Kohn-Rostoker Green's function method for defects and employ the local spin density approximation for the exchange and correlation effects. The non-spherical parts of the potential and the charge density are treated correctly, while the forces are calculated by an ionic version of the Hellmann-Feynman theorem. Lattice statics methods are used to describe the longer ranged relaxations. The calculated hyperfine fields of 5sp and 6sp elements are compared with available experimental data and it is shown that the inclusion of lattice relaxations in the calculation improves the agreement with experiments.

Relativistic ab-initio Calculations for Impurities on Surfaces

B. Nonas, R. Zeller, and P.H. Dederichs

Institut für Festkörperforschung, Forschungszentrum Jülich GmbH

T. Huhne, and H. Ebert

Institut für Physikalische Chemie, LMU München

Abstract

Under bulk like conditions the orbital moments are quenched due to strong hybridization. In consequence the lower coordination at surfaces leads not only to higher local spin moments but also to enhanced orbital contributions. This puts forward the question, whether or not a further lowering of the symmetry might increase the effects of spin-orbit interaction.

To answer this question we developed a fully relativistic KKR-Greensfunction method for surfaces and for impurities on surfaces, in which the full Dirac equation is solved in the local density approximation. We compare the results of our calculations for the spin and orbital contributions to the local magnetic moments for the Fe(001) surface to earlier studies. Furthermore we study the enhancement of the orbital moment due to the inclusion of Brooks' term for the orbital polarization. As a first study for clusters on surfaces we present here the results of calculations for single 5d impurities on and in the (001) surface of Au. Of particular interest is the reduction of the spin moments due to the spin-orbit coupling and the size of the orbital moments.

A TB-KKR Study of Magnetic Moments and Hyoerfine Fields at the Fe/Co Interface

V. Bellini, R. Zeller, P.H. Dederichs

Institut für Festkörperforschung, Forschungszentrum Jülich D-52425 Jülich, Germany

Abstract

In this work the profiles of the magnetic moments and hyperfine fields at the *bcc* Fe/Co interface for the (100) and (110) geometries are investigated by means of the Tight-binding (TB) Korringa-Kohn-Rostoker (KKR) for layered systems using the Green's-funtion approach within the Local-Spin-Density-Approximation (LSDA). We discuss the relation between the local moments and the hyperfine fields at the interface; furthermore calculations for a Cd probe atom at the interface are presented, allowing a direct comparison with TD-PAC (Time Dependent Perturbed Angular Correlation) spectroscopic experiments [1]. As expected from Fe/Co alloys studies, no oscillatory behaviour is found for the magnetic moments of Fe approaching the interface. However in contrast to this the hyperfine fields of the probe atom show oscillations around 'bulk' like values.

[1] B. Swinnen et al., Phys. Rev. Lett. **78**, 362 (1997)

A New Method to deal with Large Lattice Distortions within the KKR–Formalism

Ch. Zecha[1], A. Settels[2], R. Zeller[2], H. Ebert[1], and P. H. Dederichs[2]

[1] *Institut für Physikalische Chemie, Universität München, Theresienstr. 37, D-80333 Munich, Germany*

[2] *Institut für Festkörperforschung, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany*

Abstract

Lattice distortions have so far been dealt with in the KKR-formalism by means of a so called U–transformation. Here the shift of a lattice site is accounted for by a reexpansion of the electronic Greens function. However, the associated angular momentum series has limiting convergence properties. For that reason a new method has been developed that

allows us to treat arbitrary lattice distortions with high precision. It uses an auxiliary lattice including the shifted positions as additional sites. This method will be presented in some detail and an outlook to future applications will be given.

Screened real-space study of the magnetic properties of the transition metals.

L. Petit, S.V. Beiden, W.M. Temmerman, Z. Szotek, G.M. Stocks, and G.A. Gehring

Abstract

We have implemented screening in the fully relativistic spin-polarized version of the Korringa-Kohn-Rostoker (KKR) band-structure method. Exploiting the resulting sparsity of the KKR matrix we were able to accelerate the matrix inversions, and to study the convergence of magnetic moment and the magnetic anisotropy energy (MAE), on the central site of a local interaction zone, as a function of atoms in this zone. We show the results obtained for the magnetic moment and MAE of Fe, Co and Ni. Also we investigate the effect of lattice distortions on the MAE of fcc Co.

Magnetism, Structure and Alloy Formation of Ultrathin Films

Robert Abt and Stefan Blügel

Institut für Festkörperforschung des Forschungszentrums Jülich, D–52425 Jülich

Abstract

c$(2 \times 2)MnCu$/Cu(100) became a model system for an ordered, two-dimensional, magnetic alloy film at one monolayer thickness. LEED, STM, SARUPS, IPES (BIS), MXD, and holography have been used to investigate this alloy. The possibility of the formation of similar surface alloys have been explored: c$(2 \times 2)MnNi$/Ni(100), c$(2 \times 2)MnCu$/Cu(110), c(2×2)MnCo/Co(100), c$(2 \times 2)MnAg$/Ag(100), c$(2 \times 2)MnPd$/Pd(100), Cr/Fe(100). We investigate by first principles calculations with the FLAPW-film and bulk method, based on the density functional theory, in local spin density and the generalized gradient approximation, the energy for the alloy formation and the segregation for c$(2\times 2)3dCu$/Cu(100) surface alloys. Our investigations show a clear trend: i) Magnetism acts against interdiffusion. At low coverage, where the magnetism of Cr and Mn is very strong, interdiffusion is suppressed. ii) Magnetism reduces clustering and promotes alloy formation. From i) + ii) we expect for the case of the Cu substrate a thermodynamically stable, two dimensional surface alloy: c$(2 \times 2)MnCu$/Cu(100). Similar conclusions can be drawn for the c$(2 \times 2)MnCu$/Cu(110) and c$(2 \times 2)MnNi$/Ni(100). Investigation for the Ag and Pd substrates show a different picture due to their larger lattice constant.

Theoretical approaches of spin-electronics

P. Bruno

Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

Abstract

The emerging field of spin-electronics (or magneto-electronics) is currently attracting an increasing interest, with results from the new perperpectives it opens in for applications in information and sensor technology.

I shall first give a short survey of the various problems that are investigated experimentally and review the theoretical approaches that can be used to treat them. In particular, I shall focus on the approach based upon the "non-equilibrium Green's function" formalism, which in my view is the most versatile and promising approach. Then, I shall give a brief survey of projects in spin-electronics carried out in the Theory Department of the MPI of Microstructure Physics.

Resistivities and GMR for the MOTOROLA spin valve

C. Blaas, P. Weinberger and L. Szunyogh

Center for Computational Materials Science and Institut für Technische Elektrochemie und Festkörperchemie, Technische Universität Wien, Vienna, Austria

P. M. Levy

Department of Physics, New York University, New York, USA

C. B. Sommers

Laboratoire de Physique des Solides, Université de Paris-Sud, Orsay, France

Abstract

We have used the spin-polarized relativistic screened Korringa-Kohn-Rostoker method for layered systems together with the Kubo-Greenwood formalism and the coherent potential approximation to describe electrical transport properties of magnetic multilayers that allows us to calculate resistivities and magnetoresistance of finite systems with no adjustable parameters by simultaneously determining contributions to the giant magnetoresistance of multilayers coming from both the electronic structure and spin dependent scattering off impurities. This method is applied to study the industrial MOTOROLA spin valve, i.e., the "bottom spin valve" NiO/Co 40 Å/Cu 19 Å/Co 40 Å operating in the current in plane geometry. Our preliminary calculations predict a GMR of 12% which compares rather well with the measured 13.3%.

Spin polarization in magnetic tunnel junctions

P. Zahn and I. Mertig

Institut für Theoretische Physik, TU Dresden, D-01062 Dresden, Germany

Abstract

In recent experiments it was shown that the tunnel magnetoresistance (TMR) ratio decreases by inserting a nonmagnetic layer between the magnetic electrodes and the tunnel barrier /1/. The decay length for a coverage of Co electrodes with Al is of the order of the atomic layer distance, whereas for Cu and Ag the decay is significantly weaker.

We present ab initio electronic structure calculations which have been performed using a Screened KKR method based on DFT. We consider pure Co and Fe electrodes, and the influence of Al and Cu overlayers. The tunnel barrier was simulated by vacuum. The TMR ratio depends strongly on the spin polarization of the local density of states (LDOS) at the electrode/barrier interface. The Al overlayer causes the formation of surface states in the majority band. Consequently, the polarization is strongly reduced. In the case of a Cu overlayer no surface state formation is obtained in the majority band. The spin polarization remains nearly unchanged and the spin polarization of the LDOS decays slowly with increasing Cu thickness.

/1/ S.S.P. Parkin, private communication

Asymptotic behaviour of the Oscillatory Exchange Coupling in Magnetic Multilayers

N. N. Lathiotakis[a], B. L. Györffy[a], B. Újfalussy[b]

[a] *H. H. Wills Physics Laboratory, Royal Fort, Tyndall Ave., BS8 1TL, UK.*
[b] *Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA.*

Abstract

A model based on screened KKR-CPA method has been developed for studying the Oscillatory Exchange Coupling across binary alloy spacers. The stationary phase method is employed and an analytic asymptotic form of the coupling energy is derived. The model is used to calculate the Oscillatory Exchange coupling for all the (100), (110) and (111) growth directions of Co/Cu/Co trilayer and the results compare well with both full integration calculations over $\mathbf{k}_{||}$ and the experiment.

Domain wall resistance in ferromagnets

Arne Brataas, Gen Tatara, Gerrit E. W. Bauer, Ramon van Gorkom, Jeroen van Hoof, and Paul J. Kelly

Abstract

We study transport through ballistic and diffuse ferromagnetic domain walls. For a ballistic domain wall, the change in the conductance due to the domain wall scattering can be obtained from an adiabatic approximation valid when the length of the domain wall is much longer than the Fermi wavelength. When realistic band-structures are used, the domain wall resistance is enhanced by orders of magnitude compared to the results for a two-band Stoner model. In diffuse systems, the change in the resistivity is calculated in a two-band Stoner model using a diagrammatic technique to the lowest order in the domain wall scattering and taking into account spin-dependent scattering lifetimes and screening of the domain wall potential. The domain wall scattering causes a reduced magnetization which can give rise to a negative domain wall resistance when the scattering lifetime of the minority electrons is larger than the scattering lifetime of the majority electrons.

Bloch Wall properties from first principles calculations

J. Schwitalla and B. L. Györffy
University of Bristol

Abstract

In this talk I will present the status of our work on first principles calculations of Bloch wall properties.

We model a Bloch wall by a half infinit bulk system on the left hand side with magnetization in one easy direction a half infinit bulk system on the right hand side with magnetization in another easy direction and N layers inbetween with the magnetization linearly turning round between the two limiting directions.

The energy difference between such a configuration and the pure bulk system can then be calculated as a function of the thickness N. The minimum of the resulting curve $E(N)$ provides an estimate for the Bloch wall thickness and the Bloch wall energy.

Within the Heisenberg model $E(N)$ is given by

$$E(N) = \frac{\alpha}{N} + \beta N$$

where α is proportional to the exchange coupling parameter J and β is proportional to the anisotropy constant K.

Comparing the curve $E(N)$ obtained from the first principles calculation with the prediction from the Heisenberg model provides a test on the applicability of the latter and furthermore yields a value for J which can be compared with other independent theoretical predictions e. g. from spin wave calculations.

I will present results for bcc iron.

Simulation of the tunnel current from first principles electronic structure calculations: magnetic surfaces

W. A. Hofer and J. Redinger

CMS-Vienna

Abstract

Within a first order perturbation approach and in Bardeen's formulation the tunneling current is based on the electronic structure of the electron states of a sample surface and the STM tip. We use a newly developed numerical evaluation scheme to calculate the tunnel current above magnetic Fe(100) and PtNi(100) surfaces. It can be schown that the states of the tip influence the corrugation amplitude quite substantially, which to some extent accounts for the deviation between experimental values and calculated corrugations pertaining to the Tersoff-Hamann model.

Magnetic Surfaces under Static External Electric Fields

Stefan Blügel[†], Xiliang Nie[†], and Michael Weinert[‡]

[†]*Institut für Festkörperforschung des Forschungszentrums Jülich, D–52425 Jülich*
[‡]*Department of Physics 510A, Brookhaven National Laboratory,*
Upton, NY 11713-5000, USA

Abstract

Controlling and manipulating magnetic properties are key issues in the field of magnetic nanostructures. One possible external parameter is the static external electric field. Sizeable electric fields in the order of $\sim 10^7 \div 10^8$ V/cm can be applied by AFM or STM and can occur in contact with electrolytes in electrolytic cells. There is practically no investigation of magnetic surfaces in electric fields. In this talk we investigate the change of the magnetization direction under electric fields. We have calculated the magneto-crystalline anisotropy (MCA) energy for a couple of ultrathin films and determined the easy magnetization axis. With external electric fields we can modify the MCA which leads to interesting consequences. All results are based on the density functional theory in the local spin-density approximation and are obtained with the FLAPW-method in film geometry. The electric field and the spin-orbit interaction in the second-variational procedure was implemented. All calculations including the ones with the spin-orbit interaction have been carried out self-consistently.

STM-SPECTRA FOR TRANSITION METAL IMPURITIES ON THE FE(001) SURFACE

N. Papanikolaou, B. Nonas, Ph. Mavropoulos, R. Zeller, and P.H. Dederichs

Institut für Festkörperforschung, Forschungszentrum Jülich GmbH

Abstract

Microscopic studies using the scanning tunneling microscope have greatly enhanced our knowledge on the physical processes on metallic surfaces. One difficulty is the chemical identification of the surface atoms, since the signal recorded reflects the density of states that decay to the vacuum region. Recently a sharp feature in the tunneling spectra of the bcc (001) surfaces of Fe and Cr was discovered. This was also used to identify Cr impurities on a Fe (001) substrate [1]. Here we will present ab-initio calculations for several transition metal impurities on a Fe (001) surface. The electronic structure in the vicinity of the defect is calculated using the Korringa-Kohn-Rostoker Green's function method within the local density approximation. We first calculate the bulk Green's function, then create two half crystals by removing some atomic planes and finally embbed an impurity in the surface environment. The s-tip-model of Tersoff and Hamann is used to calculate the tunneling spectra. Our calculations agree well with the experiment for the Cr impurity. The results for other 3d impurities yielding similar peaks around E_F will be discussed.

[1] A. Davies, J.A. Stroscio, D.T. Pierce, and R.J. Celotta, Phys. Rev. Lett. **76**, 4175 (1996)

X-ray magnetic dichroism shows every atom has its moments

Gerrit van der Laan

Daresbury Laboratory, Warrington WA4 4AD, UK

Abstract

Conventional magnetism has largely ignored the anisotropy of the spin and orbital magnetic moments and so far not much is known about the factors which influence the preferred magnetization of thin films, multilayers and interfaces. Yet the ability to grow thin epitaxial films has led to materials with novel magnetic properties, such as perpendicular magnetic

anisotropy (PMA), giant magnetoresistance (GMR) and exchange biasing, with immediate technological applications. The preferred orientation of the magnetization is determined by the magnetocrystalline anisotropy energy (MAE), which is the change in the free energy of the material upon rotation of the applied magnetic field. In thin films and multilayers the MAE is usually strongly increased from the bulk due to the symmetry breaking. It is shown how the newly developed experimental tool of Transverse X-ray Magnetic Circular X-ray Dichroism (XMCD) can be used to determine the easy axis of magnetization for each constituent of a composite magnetic system. For instance, it was found that a 3 monolayer (ML) thin Co film is able to rotate the easy-direction of magnetization of a much thicker (33 ML) Ni film. [1] By applying the well known sum rule the anisotropy in the orbital moment is obtained from the integrated XMCD signal. When the spin-orbit interaction is treated in second-order, the MAE is expected to be proportional to the expectation value of the anisotropic part of the orbital magnetic moment, [2] so that in principle we have a measure for the magnetic anisotropy. However, the latter relation is only valid under specific circumstances, while in other cases there will be a proportionality factor that depends on the electronic structure of the material. There are additional terms which are related to the spin-subband orbital moment and to the magnetic dipole operator due to the anisotropy of the field of the spin. The latter term accounts for the spin-flip excitations between the exchange split majority and minority spin bands. [3] These shortcomings in the model make it necessary to search for alternative ways of measuring the magnetization preference. It is argued that X-ray Magnetic Linear Dichroism (XMLD) might be able to conduct magneticians to the holy grail of the element-specific magnetic anisotropy. [4] For itinerant 3d transition metal systems the MAE is directly related to the anisotropic part of the spin-orbit interaction which can be obtained by applying the sum rule for linear dichroism. This appliance might also be practical to dissect the MAE into the different contributions of the spin-orbit related anisotropy and the shape anisotropy due to dipole-dipole interactions.

References:

[1] H.A. Durr, G.Y. Guo, G. van der Laan, J. Lee, G. Lauhoff and J.A.C. Bland, Science 277, 213 (1997).

[2] P. Bruno, Phys. Rev. B. 39, 865 (1989).

[3] G. van der Laan, J. Phys. Condens. Matter 10, 3239 (1998).

[4] G. van der Laan, Phys. Rev. Lett. 82, 640 (1999).

Magnetic EXAFS Investigations on Fe/Cu and Fe/Co Multilayers

V. Popescu and H. Ebert

Institut für Physikalische Chemie, Universität M"unchen,Theresienstr. 37, 80333 München

Abstract

The fully relativistic theory of magnetic EXAFS (MEXAFS) developed recently by the authors, has been applied to several transition metal multilayers. For the Fe/Cu and Fe/Co multilayer systems results for the K-edges of Fe, Cu and Co will be presented and compared with available experimental data. In particular, the changes in the (M)EXAFS spectra, as a

direct consequence of the changes in the local magnetic environment, have been investigated. For this purpose, calculations for disordered alloys were performed in addition.

Theoretical x-ray magnetic circular dichroism study of the magnetic properties of Fe ultrathin films on W(110) and of $Co_{50}Pt_{50}$ thin films

I. Galanakis, M. Alouani, H. Dreyssé and J. M. Wills[†]
Institut de Physique et Chimie des Matériaux de Strasbourg, 23 rue du Loess, BP 20 CR, F-67037 Strasbourg, France
[†]*Los Alamos National Laboratory, NM 87545*

Abstract

The synchrotron radiation gives us the possibility to study the relation between the electronic structure, the magnetic anisotropy and the XMCD (X-rays Magnetic Circular Dichroism). The sum rules have become a powerful utility for the calculation of the spin and orbital magnetic moments from the XMCD spectra. We present an *ab-initio* investigation of Fe ultrathin films on W(110). The method used, FP-LMTO (full-potential linear muffin-tins orbitals method), let us relax the atomic positions and after calculate the electronic structure. In this system, it's already known that the spin magnetic moments on the atoms of Fe are more important than in the case of bulk Fe. The easy magnetization axis for one layer of Fe is in-plane, but when we add a second layer it rotates and becomes perpendicular to the surface.

The second system, that we will present, is the $Co_{50}Pt_{50}$. This system is a good candidate for magneto-optical recording units because the magnetization axis is along the [001] direction, perpendicular to the layers. For this system we calculated the XMCD spectra for different quantization axis. The calculated spectra compare well with experiments performed by W.Grange *et al.* We discuss the evolution with the spin quantization axis of the directly calculated orbital magnetic moment by our method and the one calculated by applying the sum rules to the experimental spectra. Finally a particular interest is reserved to the spin magnetic moment on Pt induced by the spin-orbit coupling and the $3d$-$5d$ hybridization.

Magnetic structure and anisotropy of ultra-thin Ni films on Cu(001) revisited

Jürgen Henk, Susanne Mirbt, Anders Niklasson, and Börje Johansson
Condensed Matter Theory Group, University Uppsala, Sweden

Abstract

Our previous calculations [1] on magnetism and anisotropy of Ni films on Cu(001) related the experimentally observed spin reorientation transition to the tetragonal distortion of the Ni film and successfully reproduced the critical film thickness of 6 mono layers (ML). However, some questions remained unanswered.

For example, at 2 ML and 3 ML thickness, we found perpendicular anisotropy, in contrast to experiments. In order to explain this disagreement, we investigated the effect of film quality [2] on the magnetic anisotropy energy (MAE).

Our results revealed further a rather strong quantum-well derived contribution to the MAE. Particularly this part of the MAE should considerably depend on the boundary conditions. For example, covering the Ni film with non-magnetic capping layers shifts the critical thickness from 6 ML to 5 ML, as observed in experiment [3].

---

[1] J. Henk, A. M. N. Niklasson, and B. Johansson, Phil. Mag. B = **78**, 585 (1998); Phys. Rev. B **59** (1999), in press.

[2] W. Platow, A. N. Anisimov, G. L. Dunifer, M. Farle, and K. = Baberschke, Phys. Rev. B **58**, 5611 (1998).

[3] W. L. O'Brien, T. Droubay, and B. P. Tonner, Phys. Rev. B = **54**, 9297 (1996).

Calculating interface reflection and transmission matrices from first-principles using localized-orbital bases

K. Xia, P.J.Kelly, G.E.W. Bauer, J. Kudrnovsky, and V. Drchal

Abstract

A study of transport in magnetic multilayers based on the Landauer-Bűttiker formalism requires the calculation of interface reflection and transmission matrices. In an earlier study of the interface resistance of Co/Cu multilayers, we obtained these matrices from a formulation of the embedding method in terms of transfer matrices. The disadvantage of this procedure, which was based on the FLAPW method, was that calculations for even small unit cells were computationally very expensive. Here we explore the possibility of calculating reflection and transmission matrices using minimal localized-orbital bases such as the TB-LMTO.

Spin density waves in Cr films

L. Nordstrom

Abstract

The magnetic profile of Fe/Cr_N/Fe bcc(001) films has been calculated by means of first principles density functional theory. It is shown that the magnetic profile of the chromium spacer can be expressed in terms of spin density waves (SDW). The dispersion and amplitude of the SDW are determined and the effects from the finite film thicknesses are observed and discussed. It is found that the SDW wave vectors are quantized and that for certain Cr thicknesses two SDWs with different wave lengths coexist. Connections to the magnetic interlayer coupling are discussed.

Ab initio Calculations Of Angle-Resolved Photoemission

A. Ernst, M. Lüders, A. C. Jenkins, W. M. Temmerman, Z. Szotek, and P. J. Durham

Daresbury Laboratory, Warrington WA4 4AD, UK

Abstract

We has used our recently developed angle-resolved photoemission codes to study surfaces of fcc Cu(100), Cu(110), Cu(111), and quantum well states in Cu/Co(100). The advantages of our codes are that one-electron potential functions and angle-resolved photoemission spectra are obtained by multiple scattering theory and within the same code. The calculated photoemission spectra for these three faces of Cu are in agreement with experiments. For Cu on Co(100) we could identify the quantum well states in the photoemission spectra.

Fully relativistic spin-polarized calculations of magneto-optical properties for thin films

L. Szunyogh

Center of Computational Materials Science, Vienna, Austria

Department of Theoretical Physics, Technical University Budapest, Hungary

P. Weinberger

Institute for Technological Electrochemistry, Technical University Vienna, Austria

Center of Computational Materials Science, Vienna, Austria

Abstract

A method to calculate the magneto-optical conductivity tensor of thin films as based on the Kubo-formula and the fully relativistic spin-polarized Screened KKR technique is presented. Technical developments concerning in particular the occurring energy integration are discussed. The numerical stability of the method will be demonstrated. An extension of the calculations to statistically disordered alloy films is also pointed out. Our first application concerns Co/Pt overlayers, where a considerable enhancement of a perpendicular magnetic anisotropy has already been found.

Understanding of Invar effect in Fe-Ni alloys

I. A. Abrikosov[†], Mark van Schilfgaarde[*], and B. Johansson[†]

[†] *Condensed Matter Theory Group, Physics Department,*
Uppsala University, S-75121 Uppsala, Sweden
[*] *Sandia National Laboratories, Livermore, California 94551, USA*

Abstract

We present results of *ab initio* calculations of magnetic and thermodynamic properties of a random fcc Fe-Ni Invar alloy, where we allow for noncollinear spin alignments. The alloy is modeled by a supercell of 32 atoms. We find that the transition from the high-volume high-spin state to the low-volume low-spin state proceeds as a continuous transition to a disordered noncollinear configuration. The noncollinearity gives rise to an anomalous volume dependence of the binding energy curve, and explains the well-known peculiarities of Invar systems.

Interfacial alloying at the Cr/Fe(001) interface: influence of the chemical order on the magnetic order

M. Freyss, D. Stoeffler, H. Dreyssé
IPCMS, 23 rue du Loess, 67037 Strasbourg, France.
I. Turek, P. Weinberger,
Center for Computational Materials Science, Gumpendorferstrasse 1a, 1060 Wien, Austria.

Abstract

We present the results of our theoretical study of the magnetic order in Cr films on a Fe(001) substrate taking into account interdiffusion at the interface. It has been shown experimentally that a strong interdiffusion occurs at the Cr/Fe(001) interface. In our calculations, we discuss its influence on the overall magnetic properties of the system. Interdiffussion in modelled by two monolayers of FeCr alloy at the interface, whose concentration is varied. Two cases have been considered: an interfacial ordered alloy on the one hand, and a fully disordered alloy on the second hand. The magnetic order is then respectively determined by means of a semi-empirical real-space TB model, and by means of the *ab-initio* CPA-TB-LMTO method. We find that the magnetic properties of the Cr films is very similar with both types of alloy, suggesting very little influence of the chemical order on the magnetic order of the system. We show that only a weak interdiffusion is needed to reverse the phase of the layer-by-layer antiferromagnetic order of the Cr films, and thus obtain a magnetic structure in accordance with experimental data.

A Fully Relativistic Description of Spin-Resolved Auger Emission Spectroscopy

J. Minár, V. Popescu and H. Ebert

Institut für Physikalische Chemie, Universität München, Theresienstr. 37, D-80333 Munich, Germany

Abstract

We present a theoretical description of the spin-resolved Auger emission spectroscopy (SR-AES) that has been setup within the framework of relativistic multiple scattering theory, on the basis of Dirac equation for spin-polarized, magnetic solids. This approach allows one to investigate the core-core-core (CCC), the core-core-valence (CCV) as well as the core-valence-valence (CVV) SR-AES for paramagnetic and ferromagnetic transition metal systems. Several applications for the CVV-case are presented and compared with available experimental data.

Calculation of magneto-optical properties of layered systems by means of the SPR-KKR-method

T. Huhne, and H. Ebert

Institut für Physikalische Chemie, Universität München, Theresienstr. 37, 80333 München, Germany

e-mail: he@gaia.phys.chemie.uni-muenchen.de

Abstract

The comparison of experimental and theoretical magneto-optic spectra of magnetic solids in the visible regime is of considerable interest for the understanding of the electronic structure of solids. Within this field, the main interest lies on the magneto-optic Kerr-effect (MOKE), which nowadays is also used in magneto-optic storage technology using magnetic multilayer- and surface layer systems whith increasing success.

On the basis of the fully relativistic self consistent spin-polarised Green's function method (FPSPRKKR) for the ab-initio-calculation of the electronic structure of multilayer- and surface layer systems, which was presented earlier, we have developed and implemented a calculational method to determine the frequency-dependent, layer resolved optical conductivity tensor. The optical conductivity privides a bridge to calculate all experimentally accessible magneto-optical quantities like Kerr rotation angles within a classical formalism based on macroscopic Maxwell equations.

First results for the layer resolved optical conductivity and the MOKE of transition metal bulk crystals (Fe and Co) are presented and compared to experimental results and to calculations of other authors. Emphasis will be laid – as a new feature of such calculations – on the layer-resolved magneto-optical properties.

Residual resistivity in Ni_xCr_{1-x} and Ni_xCu_{1-x} fcc-alloy systems

A. Vernes and H. Ebert

Institut für Physikalische Chemie, Universität München, Theresienstr. 37, D-80333 München, Germany

J. Banhart

Fraunhofer-Institut für Angewandte Materialforschung, Lesumer Heerstr. 36, D–28717 Bremen, Germany

Abstract

First-principles calculations of the electrical resistivity of disordered alloys based on the Kubo-Greenwood formalism and the spin-polarized Korringa-Kohn-Rostoker coherent-potential-approximations are presented. Application to the fcc alloy systems Ni_xCr_{1-x} and Ni_xCu_{1-x} yields results for the residual resistivity and critical concentration (concentration for which the paramagnetic-to-ferromagnetic phase transition takes place), respectively, in

very satisfying agreement with experiment. In addition, scalar-relativistic calculations were performed on the basis of the two-current model for these alloy systems. For the paramagnetic phase these were found to be in better agreement with the experiment than the fully relativistic results.

Relativistic Scattering Theory of Magnetisation-Induced Second Harmonic Generation

E. Arola [a], S. Crampin [a], L. Calmels [b], and J. E. Inglesfield [b]
[a] *University of Bath, Department of Physics, Bath BA2 7AY, UK*
[b] *Department of Physics and Astronomy, University of Wales, Cardiff CF1 3XP, UK*

Abstract

Magnetisation Induced Second Harmonic Generation (MSHG) technique is a powerful non-linear magneto-optical tool for investigating surface and especially interface related magnetism. In a typical MSHG experiment the sample surface is illuminated with a linearly polarised laser beam of frequency ω and the polarisation state and intensity of the emitted 2ω signal is detected. This signal is sensitive to the electronic, magnetic, and structural properties of interfaces in the sample. We describe the outline of our first-principles theory of magnetisation-induced second harmonic generation for surfaces and planar interfaces of materials. The theory is based upon the time-dependent second order perturbation theory and will be implemented within the fully relativistic, spin-polarized layer-KKR multiple-scattering method (R-SP-LKKR). This approach enables a realistic treatment of buried interfaces and multilayers, and we also describe how screening of the incident and second harmonic field can be treated within our framework.

Calculation of magnetic X-ray emission dichroism in disordered Co-Rh-based ternary alloys

S. Ostanin

Abstract

Fully relativistic investigations on the magnetic circular dichroism in absoption and emission have been performed for Rh in the alloy systems $\mathrm{Co}_{0.75}\mathrm{Rh}_{0.25}$, $\mathrm{Co}_{0.75-x}\mathrm{Rh}_{0.25}\mathrm{Ni}_x$ and $\mathrm{Co}_{0.75}\mathrm{Rh}_{0.25-x}\mathrm{Pd}_x$. The results obtained using the spin-polarized relativistic Korringa-Kohn-Rostoker method of band structure calculation together with the Coherent-Potential-Approximation (SPR-KKR-CPA) allow one a detailed interpretation of corresponding experimental data. The changes for the magnetic moments of Co and Rh in the binary alloy $\mathrm{Co}_x\mathrm{Rh}_{1-x}$ caused by substitution of Rh by Pd and Co by Ni, respectively, are discussed in comparison with experimental data and a generalized Slater-Pauling curve.

Fully relativistic calculations of the spin- and orbital susceptibility and Knight-shift in homogeneous and non-homogeneous systems

H. Freyer, M. Deng and H. Ebert

Institut für Physikalische Chemie, Universität München,
Theresienstr. 37, D-80333 München

Abstract

In the framework of the spin–polarized, relativistic KKR–Green's function method we implemented the linear response formalism in order to calculate local magnetic susceptibilities and Knight shifts in homogeneous as well as inhomogeneous systems taking into account properly all spin– and orbital contributions. Corresponding calculations are presented for bulk d–transition metals and for the layer–resolved (001)–surface of fcc-Pt showing pronounced differences between the results for the bulk and the surface layers in the latter case.

Relativistic Photoemission for magnetic and non-magnetic metallic surface

Matthew Woods

Abstract

An outline of the theory of relativistic photoemission will be presented and a cluster code will be described. Ongoing calculations (based on real space KKR) for Cu(100) will be compared with experimental results and non-relativistic calculations.

Theoretical study of the magnetic properties of different supported nanostructures

J. Izquierdo, R. Robles, and A. Vega

Departamento de Física Teórica, Atómica, Molecular y Nuclear
Universidad de Valladolid, E-47011 Valladolid, Spain

Abstract

We present theoretical results for the magnetic properties of various transition metal supported nanostructures recently characterized experimentally by STM technique, in particular Co islands on Cu and Co nanowires on Pd. The local magnetic moment distribution, average magnetization and magnetic interaction between the supported nanostructures, have been determined by solving a selfconsistent spd band model Hamiltonian in the real space. A superparamagnetic configuration is found to be stable for relatively large substrate coverage. The possible implications of this study are discussed.

Magnetic properties of 5d-impurities in bcc-Fe

M. Deng, C. Kornherr, C. Zecha, T. Huhne, H. Ebert, B. Nonas, R. Zeller, and P. H. Dederichs

Abstract

The magnetic properties of 5d-impurities in bcc-Fe have been studied by the spin-polarized relativistic version of the SPR-KKR-GF-bandstructure method. When determining the relativistic scattering path operator $\underline{\tau}$ of a ferromagnetic host system, it is possible to reduce the

calculational effort by using its transformation properties under the magnetic point group for a given direction of the magnetisation. By use of the Dyson equation connecting the $\underline{\tau}$-matrix of the perturbed system on the one hand and the $\underline{\tau}$-matrix of the host system and the single-site t-matrices of both systems on the other, the Green's function of the perturbed system and thereby all interesting electronic properties of the impurity system can be calculated.

By use of a program developed on the basis of the described method, results for the spin and orbital magnetic moments and hyperfine fields of 5d-transition metal impurities in Fe have been obtained.

"Local moments" and electronic structure of Fe films above the Curie temperature

S.S.A. Razee and J.B. Staunton

Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom

L. Szunyogh

Department of Theoretical Physics, Technical University of Budapest, Budapest, Hungary
and Centre for Computational Materials Science, Wien, Austria

B.L. Gyorffy

H.H. Wills Physics Laboratory, University of Bristol, Bristol BS8 1TL, United Kingdom

B. Ujfalussy

Oak Ridge National Laboratory, Oak Ridge, TN 37381, USA
and Research Institute for Solid State Physics, Hungarian Academy of Sciences, Budapest, Hungary

Abstract

Understanding the magnetic properties of two-dimensional systems such as thin films and multilayers is important both from the fundamental as well as technological point of view. At T=0 K, we have a fairly satisfactory description of these properties from first-principles electronic structure calculations. However, at finite temperatures, in particular above the Curie temperatures, there is very little work. There are many exotic and interesting observations which needs to be explained in terms of an ab initio theory. In this talk we present a scheme based on the disordered local moment (DLM) picture to study the temperature dependence of magnetic properties of thin films. We demonstrate the applicability of the DLM theory to thin films by studying the fcc-Fe films on Ag(001) substrates.

Spin polarization at Fe/V and Co/Cr interfaces

J. Izquierdo, A. Vega

Departamento de Física Teórica, Atómica, Molecular y Nuclear
Universidad de Valladolid, E-47011 Valladolid, Spain

C. Demangeat

Institut de Physique et Chimie des Matériaux de Strasbourg, 23, rue du Loess, F-63037 Strasbourg, France

Abstract

The spin polarization at the Fe/V and Co/Cr interfaces is investigated using the tight-binding linear muffin-tin orbital (TB-LMTO) method.

In the case of Fe/V we consider both Fe_nV_m superlattices and thin V_m films on Fe substrates in the (100) and (110) orientations. We obtain a short-range induced spin-polarization in V, as well as reduced Fe polarization at the Fe/V interface. In Fe_nV_m superlattices, V couples always antiferromagnetically with Fe. For thin V films grown on Fe(100) the V polarization presents oscillations (layered antiferromagnetic configuration). The magnetic moments of V and Fe depend on the crystallographic orientation of the sample. Our results are compared with the existing experimental observations.

For Co/Cr systems we have studied thin Co_m films on Cr substrate for (100), (110) and (111) orientations, in order to clarify how the magnetic profiles of the system depend on the crystallographic orientation.

Structural and electronic properties of $Cu_xZn_yAl_{100-x-y}$

V.Crişan[a],H.Ebert[a],H.Akai[c],P.Entel[b]

[a] *Institut für Physikalische Chemie, Universität München, Theresienstr. 37, 80333 München*

[b] *Theoretische Physik, Gerhard-Mercator-Universität Duisburg,47048 Duisburg*

[c] *Department of Physics, Osaka University, 1-16 Machikaneyama, Toyonaka, Osaka 560, Japan*

Abstract

Structural instability, spinodal decomposition, and rubber-like behavior at different compositions are discussed on the basis of energy surfaces for energy differences between various crystal structures, for mixing energies, for spinodal decomposition, and for electronic densities of states at the Fermi energy. The results show that one can discuss the stability of different phases on the basis of energy differences and mixing energies. Results for the density of states confirm to a certain extent the phenomenological Hume-Rothery rules. In the high Cu concentration limit the system are showing short range ordering tendency with nesting vectors in [100] and [110] directions of the Brillouin zone.

The effect of magnetism on the vacancy formation energy in 3d metals

P. A. Korzhavyi, I. A. Abrikosov, and B. Johansson

Condensed Matter Theory Group, Uppsala University, S-75121 Uppsala, Sweden

Abstract

The vacancy formation energy in the 3d, 4d, and 5d transition and noble metals have been calculated from first principles using the order-N, locally self-consistent Green's function

method in conjunction with a supercell approach. The calculations include electrostatic multipole corrections to the atomic sphere approximation. The results are in excellent agreement with experiment and existing full-potential calculations. The effects of crystal and magnetic structure on the vacancy formation energy are analysed in terms of the local changes of the electron state density induced by the vacancy.

3.1.2 Report on the Hands-On Dichroism Course

A Hands-On Dichroism Course was held in Daresbury Laboratory from Monday, April 26, until Thursday, April 29. The purpose of the course was to teach experimentalists the use of band structure computer codes for generating the self-consistent one-electron potentials and with them to calculate the X-ray absorption and dichroism spectra. The self-consistent LMTO band structure code and the dichroism code were nicely interfaced with the plotting programmes, allowing the participants to see density of states, X-ray absorption and dichroism spectra, and the Kerr angle spectra, on their screens. The course was organised with lectures in the morning and practical sessions in the afternoon. The full programme is attached below. Seven teams, consisting on average of two or three students and one teacher, were formed. During the practical sessions each team was running the codes starting with well known examples such as iron, cobalt, nickel, and FeCo. After that more complicated systems such as multilayers, magnetites (Fe_2O_3), US, and others, were tackled with a varying rate of success. All teams' progress and findings were then discussed in the daily, morning team-report sessions. Some of the more complicated examples revealed some limitations of the codes and required additional changes to the codes, which were dealt with either during the practical sessions or postponed till later stage. Since the course, most problems have been fixed and most updated versions of the codes are available by annonymous ftp from:

`olymp.cup.uni-muenchen.de`

in the directory

`pub/akhe/tmr/` .

The course had a very lively atmosphere and gave the participants a very good idea of how bandstructure calculations work and how to apply the codes to generate the relevant spectra of interest. It also helped the developers of the codes in identifying any possible problem that needed fixing.

Final Programme

Monday 26th	
10:00 - 11:00	M. Brooks ”*LMTO I*”
11:00 - 11:30	Coffee
11:30 - 12:30	M. Brooks ”*LMTO II*”
12:30 - 14:00	Lunch
14:00 - 18:00	SCF-Calculations
Tuesday 27th	
9:00 - 10:00	H. Ebert ”*Relativistic Spectroscopy I*”
10:00 - 10:30	Coffee
10:30 - 11:30	H. Ebert ”*Relativistic Spectroscopy II*”
11:30 - 12:30	Team Reports
12:30 - 14:00	Lunch
14:00 - 18:00	SCF-Calculations
Wednesday 28th	
9:00 - 10:00	P. Strange ”*Relativistic DFT*”
10:00 - 10:30	Coffee
10:30 - 11:30	M. Brooks ”*Orbital Polarization*”
11:30 - 12:30	Team Reports
12:30 - 14:00	Lunch
14:00 - 18:00	SCF-Calculations
Thursday 29th	
9:00 - 10:00	P. Strange ”*Magnetic X-ray Scattering*”
10:00 - 10:30	Coffee
10:30 - 11:30	G. van der Laan ”*Sum Rules*”
11:30 - 12:30	Team Reports
12:30 - 14:00	Lunch
14:00 - 18:00	SCF-Calculations

The list of participants, including the teachers:

Gisele Benayoun (*ESRF, Grenoble Cedex*)
Peter Jan Bode (*University of Cambridge, Cambridge*)
Mike Brooks (*Forschungszentrum Karlsruhe, Karlsruhe*)
Ming Deng (*University of München, München*)
Sarnjeet Dhesi, (*CLRC, Daresbury*)
Esther Dudzik (*CLRC, Daresbury*)
Hubert Ebert (*University of München, München*)
Lars Fast (*University of Würzburg, Würzburg*)
Eberhard Goering (*Universitaet Wuerzburg, Wuerzburg*)
Robert Horny (*University of Augsburg, Augsburg*)

Ceri Jenkins (*CLRC, Daresbury*)
Gerrit van der Laan (*CLRC, Daresbury*)
Karsten Litfin (*Institute for Transuranium Elements, Karlsruhe*)
Martin Lüders (*CLRC, Daresbury*)
Miguel Marques (*University of Würzburg, Würzburg*)
Sean Mcphail (*University of Cambridge, Cambridge*)
Peter Morall (*University of Manchester, Manchester*)
Robert Pettifer (*University of Warwick, Warwick*)
Roberto Robles (*Universidad de Valladolid, Valladolid*)
Dzidka Szotek (*CLRC, Daresbury*)
Walter Temmerman (*CLRC, Daresbury*)
Carlos A. F. Vaz (*University of Cambridge, Cambridge*)
Andras Vernes (*University of München, München*)
Andreas Vetter (*University of Würzburg, Würzburg*)

3.2 Job Announcements

POST-DOCTORAL POSITION

Philips Research Laboratories Eindhoven, The Netherlands

Interface Magnetism: Giant Magnetoresistance

Candidates are invited to apply for a post-doctoral position* to work on the theory of Giant Magnetoresistance (GMR) with the Dutch partners of the Network *Ab-initio Calculations of Magnetic Properties of Surfaces, Interfaces and Multilayers* sponsored by the European Union's Training and Mobility of Researchers programme.

The aim of the theoretical work is to bridge the gap between realistic ab-initio descriptions of the electronic structure in layered magnetic materials (P.J. Kelly: University of Twente and Philips Research Laboratories Eindhoven) and phenomenological transport models of GMR (G.E.W. Bauer: Delft University of Technology) . Candidates should have considerable experience of first-principles electronic structure calculations. Knowledge of tranport theory would be very welcome but is not a prerequisite.. The post-doc. will have the opportunity to participate in a number of collaborations with experimentalists in Eindhoven, Delft and Twente as well as with other non-Dutch nodes of the Interface Magnetism network. The research position is expected to be based in Enschede (Twente) and maintain intensive contact with Delft and Eindhoven.

Applications should be sent to
Prof. P.J. Kelly,
Faculty of Applied Physics,
University of Twente,
P.O. Box 217,
7500 AE Enschede,
The Netherlands

Additional information may be obtained from:

p.j.kelly@tn.utwente.nl, Tel.: +31-53-4893166, Fax: +31-53-4892910 or
bauer@duttnto.tn.tudelft.nl, Tel.: +31-15-2784719, Fax: +31-40-2781203

* Only nationals of Member States or Associated States of the EU (but not the Netherlands) are eligible for the position allocated to the Dutch node.

4 News from the TMR2 Network

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

4.1 Job Announcements

POST-DOCTORAL POSITION AT THE UNIVERSITY OF WÜRZBURG

Applications are invited for a 2-years postdoctoral position in the area of electronic structure theory of superconductors. The position is funded by the European Ψ_k network as part of the Training and Mobility of Researchers (TMR) programme.

The applicant will be involved in first-principles electronic-structure calculations of the superconducting state of matter. The aim is to predict materials-specific properties of superconductors, including the High-Tc compounds, on the basis of the density functional theory for superconductors. The project includes the development and implementation of new exchange-correlation functionals as well as the investigation of relativistic effects in superconductors. The candidate should have profound experience with Kohn-Sham-based band-structure calculations. Besides that, knowledge in the field of superconductivity is welcome (but not a prerequisite).

The position will be based at the Institute for Theoretical Physics of the University of Würzburg, Germany. The project is carried out in close collaboration with research groups at the University of Bristol, the Max-Planck-Institute for Solid-State Research in Stuttgart and the Daresbury Laboratory. Several visits to these reseach centres are anticipated.

Due to TMR regulations, the candidate must be of EU nationality (or from Iceland, Israel, Liechtenstein or Norway) excluding, however, German nationals and EU nationals who have resided in Germany for more than 18 months during the past 2 years. The applicant should not be older than 35.

Interested individuals should send their application by June 30, 1999, to:

Prof. E.K.U. Gross
Institut für Theoretische Physik
Universität Würzburg
Am Hubland
D-97074 Würzburg
Germany
Phone: ++49-931-888-5724
Fax: ++49-931-888-5141
e-mail: gross@physik.uni-wuerzburg.de

5 News from the ESF Programme

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

5.1 Reports on Workshops

5.1.1 Report on Workshop on Hydrogen in Semiconductors

April 14 -17, 1999, Exeter, UK

Organiser: R. Jones

Co-sponsored by the European Science Foundation through the Ψ_k network and EPSRC through the CCP9 network

The workshop was attended by 47 people with 5 from the Netherlands, 3 from Hungary, 3 from Denmark, 1 from France, Portugal and Sweden, 22 from the UK, 4 from Belarus, 3 from Germany, and 4 from the USA. There were a substantial number of post-graduate and young researchers present. Eleven theoretical groups and eleven experimental ones participated with the remit to inform each other of the latest problems and results.

There was a generous time for the invited talks (usually 45 minutes) followed by 15 minutes for discussion. The quality of the talks was such that in every case the full discussion period was needed.

The talks were given by Watkins (USA), who opened the conference with a fine review of magnetic resonance experiments on hydrogen in Si and GaAs and emphasised the amount of information to be learnt from muon studies. This was followed up by a stimulating talk by Cox (RAL) on muon studies. It seems that the hydrogen community has drifted away from the muon one in recent years and it was timely to remind the groups of advances. Ammerlaan (Netherlands) described EPR experiments on double donors complexed with hydrogen. Infrared absorption studies were described by Stavola (USA) and Bech Nielsen (Denmark). These have given theorists a lot of problems especially in the structure and properties of hydrogen molecules in Si. Murin (Belarus) described how hydrogen interacted with radiation defect while Weber (Germany) and Peaker (UK) recounted the information to be found by DLTS studies on transition metal - hydrogen defects. Clerjaud (France) noted that FTIR studies gave strange structures for passivated donors and illustrated it for S in GaP.

These experimental talks obviously give lots of problems for the theorists. Van de Walle (USA) described the huge amount of detailed information on H that comes from *ab initio* methods while Estreicher (USA) gave a talk on molecular dynamics investigations of radiation defects complexed with hydrogen. Deak (Hungary) described defects in SiC linked with hydrogen along with models for optical centres in Si, while Hourahine (UK) described the interaction of hexavacancies with hydrogen. Coomer (UK) gave a talk on the electrical levels of radiation defects which had complexes with hydrogen. Stockbro (MCI) gave a very interesting talk on STM stimiulated desorption of hydrogen from a Si surface. All these talks, created a great deal of comment from the appreciative audience.

There was also a spirited poster session with contributions from a very large number of groups.

The workshop had succeeded in bringing together various groups; alerting theorists to the problems faced by experimental groups and informing the experimental groups of the type of quantities that theory can now be calculate.

The programme and abstracts of the Workshop are given below.

Thursday April 15

07:30–08:30	Breakfast: Birks Hall
09:00–09:15	Welcome (Harrison Building)

Session I – Chairman: P. Deák

09:15–09:40	*Glimpses of hydrogen in silicon via magnetic resonance studies,* G. D. Watkins
09:40–09:50	Discussion
09:50–10:20	*Optically active hydrogen dimers in Si*, B. Hourahine, R. Jones, A. N. Safonov, S. Öberg, P. R. Briddon, and S. K. Estreicher
10:20–10:30	Discussion
10:30–11:00	Coffee
11:00–11:45	*Microscopic properties of hydrogen-containing defects in Si from uniaxial stress studies of their vibrational spectra*, M. Stavola
11:45–12:00	Discussion
12:00–12:45	*Hydrogen interacting with intrinsic defects in Si*, S. K. Estreicher, J. L. Hastings, M. Gharaibeh and P. A. Fedders
12:45–13:00	Discussion
13:00–14:00	Buffet Lunch: Harrison Building, Rms. 101–103

Session II – Chairman: B. Bech Nielsen

14:00–14:45	*Interactions of hydrogen with silicon and consequences for devices*, C. G. Van de Walle
14:45–15:00	Discussion
15:00–15:45	*Energy levels for muonium in Si and Ge and electrical activity at high temperatures*, S. F. J. Cox, R. L. Lichti, K. H. Chow, E. A. Davis, T. L. Estle, B. Hitti, E. Mytilineou, C. Schwab, A. Amato, A. Schenck, M. Charlton and P. Donnelly
15:45–16:00	Discussion
16:00–16:30	Tea
16:30–17:15	*Effect of hydrogen on thermal donor formation in silicon*, L. I. Murin, V. P. Markevich, J. L. Lindström and T. Hallberg
17:15–17:30	Discussion
18:00–19:00	Poster Session: Birks
19:30–20:15	Reception: Reed Hall
20:15–24:00	Conference Dinner: Reed Hall

Friday April 16

07:30–08:30	Breakfast: Birks Hall

Session III – Chairman: S. K. Estreicher

09:00–09:45	*Hydrogen–defect complexes in silicon: Fact and speculation*, B. Bech Nielsen
09:45–10:00	Discussion
10:00–10:45	*Electrical properties of transition metal–hydrogen complexes in silicon*, J. Weber
10:45–11:00	Discussion
11:00–11:20	Coffee
11:20–12:00	*Defect profiles and the Feklisova-Yarykin conjecture*, J. Coomer, A. Resende, R. Jones, S. Öberg and P. R. Priddon
12:00–12:15	Discussion
12:15–12:50	*Acceptor-like hydrogen dimers in silicon*, B. Aradi and P. Deák
12:50–13:00	Discussion
13:00–14:00	Buffet Lunch: Harrison Building, Rms. 101–103

Session IV – Chairman: J. Weber

14:00–14:45	*Laplace transform DLTS studies of gold–hydrogen defects in silicon*, A. R. Peaker, J. Evans-Freeman and L. Dobaczewski
14:45–15:00	Discussion
15:00–15:45	*Electric field dependent structural and vibrational properties of the* $Si(100)-H(2\times1)$ *surface and its implications for STM induced hydrogen desorption*, K. Stokbro
15:45–16:00	Discussion
16:00–16:30	Tea
16:30–17:15	*Hydrogen-passivation of double donors in silicon: atomic and electronic structure*, P. T. Huy, C. A. J. Ammerlaan and T. Gregorkiewicz
17:15–17:30	Discussion
17:30–18:15	*Complexes of Group-VI Donors with hydrogen in GaP*, B. Clerjaud, D. Côte and W. Ulrici
18:15–18:30	Discussion
19:30–20:30	Dinner: Birks Hall
20:30–	Poster Session and Bar
20:00–23:00	Bar in Birks Hall

Abstracts

SI.1: Glimpses of hydrogen in silicon via magnetic resonance studies

G. D. Watkins

Department of Physics, Lehigh University, Bethlehem, PA 18015, USA
E-mail: `gdw0@Lehigh.EDU`

Magnetic Resonance studies have supplied several important bits of information concerning hydrogen in silicon, a few of which will be described. 1) A Pt–H_2 pair formed when substitutional Pt traps two hydrogen atoms has been successfully studied by electron paramagnetic resonance (EPR). Combined with local vibrational mode (LVM) studies, a rather complete picture of its lattice and electronic structure has emerged. 2) EPR studies of neutral bond-centered hydrogen ($\mathrm{H}^0_{\mathrm{BC}}$) by Gorelkinskii and Nevinny have measured the reorientation kinetics of the defect in its positive charged state. Reorientation is equivalent to a single diffusion jump, and the remarkable observation is that the results extrapolate accurately to the high temperature diffusion measurements made many years ago by Van Wieringen and Warmoltz, $\sim$ 18 decades away! A tempting conclusion is that diffusion over this wide temperature range is dominated by the defect in its positive charged state. 3) This conclusion is surprising, however, when one looks at what has been learned from muon (μ) studies in GaAs. There, μ (a light isotope of H) takes on all of the same configurations in the lattice as in silicon, and with similar relative stabilities, but detailed (SR studies have concluded that by far the most mobile species (by a factor of $\sim 10^{10}$ at room temperature) is the neutral defect in its metastable tetrahedral site (μ^0_{T}). 4) μSR studies in silicon have been able to estimate the electron emission and conversion kinetics from and between the various charge states of the two configurations and construct an almost complete configurational coordinate diagram for the defect. Almost complete because the energy difference between the neutral defect in the BC and H configurations remains undetermined, with the question of negative-U still uncertain. This uncertainty arises from the observation again in this study of the importance of metastable $\mathrm{H}^0_{\mathrm{T}}$, in this case in the emission and conversion kinetics. This may also turn out to be important in the interpretation of the electrical studies for hydrogen.

SI.2: Optically active hydrogen dimers in Si

B. Hourahine, R. Jones, A. N. Safonov[†], S. Öberg[‡], P. R. Briddon[§] and S. K. Estreicher[♮]

School of Physics, University of Exeter, Exeter EX4 4QL
[†] Department of Physics, University of Durham, South Road, Durham DH1 3LE
[‡] Department of Mathematics, University of Luleå, Luleå S95187, Sweden
[§] Department of Physics, University of Newcastle upon Tyne, Newcastle upon Tyne NE1 7RU
[♮] Physics Department, Texas Tech University, Lubbock, TX 79409-1051, USA
E-mail: `bh@excc.ex.ac.uk`

Photoluminescence experiments on silicon soaked in hydrogen, with subsequent irradiation and heat treatment, have revealed several optical centres with exceptionally low exciton binding energies. Studies using H and D mixtures demonstrated that some of these centres contain two hydrogen atoms: both ground and excited excitonic states in B_{41} and B^1_{71} are each split into three and four lines respectively showing that the defects contain *equivalent* and *inequivalent* pairs of hydrogen atoms. Magnetic field investigations demonstrate that these centres have trigonal symmetry. Other centres, such as B^1_{81} and B^1_{18} also contain two H atoms but have C_{1h} symmetry, while others B_{80} and B^1_{19} contain three and four H atoms respectively without any symmetry.

The high symmetry of B_{41} and B^1_{71} strongly restricts possible structures of the defects, particularly in the case of B_{41}, which although it is usually reported as possessing C_{3v} symmetry, actually requires the higher D_{3d} or D_3 symmetries necessary for equivalent hydrogen atoms. There are few defect structures with such high symmetry in silicon. If the defect possesses D_{3d} or D_3 symmetry, then here are only two sites in the diamond lattice at which the centre of the defect can sit. These are the bond-centre and hexagonal lattice sites. The obvious structure, consisting of two anti-bonded hydrogen atoms attached to the pair of silicon atoms surrounding a bond centred site must be discounted, since such defects should be stable only at low temperatures.

The combined requirements of creation by irradiation and high thermal stability point towards a multivacancy–hydrogen complex. V_1 to V_5 can be excluded as these are not trigonal. As V_6 is centred on the hexagonal site and has D_{3d} symmetry, a plausible candidate is a complex between V_6 and hydrogen. From a consideration of the formation and stability of V_n defects with $n < 6$, V_6 is expected to form in irradiated material which is heated to $> 200\,^{\circ}$C.

Ab initio cluster calculations (AIMPRO) on V_6H_2 reveal that the stable defect involves an unexpected reconstruction (see cover). The properties of this complex are entirely consistent with the B_{41} centre. We therefore propose that this defect is responsible for the 1.1509 eV luminescence. Alternative structures are suggested for B^1_{71} and other H centres.

The calculations imply that the precursor, V_6, should also be optically active. It is suggested that this is the B^4_{80}, or J centre (1.107 eV), which forms in irradiated hydrogen-free material around 300–480 °C and is known to be trigonal. Stress alignment studies imply that it is vacancy related. These calculations suggest that the lowering in exciton binding energy arises from the release of tensile strain in the multi-vacancy defect consequent upon H attack.

SI.3: Microscopic properties of hydrogen-containing defects in Si from uniaxial stress studies of their vibrational spectra

Michael Stavola

Department of Physics, Lehigh University, Bethlehem, PA 18015, USA
E-mail: `mjsa@Lehigh.EDU`

Vibrational spectroscopy has been an especially fruitful method for the study of hydrogen-containing complexes in semiconductors. The hydrogen vibrational bands provide an important fingerprint of the hydrogen-containing complexes, isotope shifts help identify the atoms in the complexes, and the vibrational frequencies are an important benchmark for theory. Uniaxial stress perturbations, when used in conjunction with vibrational spectroscopy, provide additional information about the microscopic properties of the defects. In favorable cases, the symmetry, reorientation kinetics, and ground state energy shift can be determined, revealing interesting physics that is not accessible to vibrational spectroscopy alone. The BH, AuH_n, and H_2 centers in Si will be discussed as examples.

SI.4: Hydrogen interactions with intrinsic defects in Si

S. K. Estreicher, J. L. Hastings, M. Gharaibeh and P. A. Fedders [†]

Physics Department, Texas Tech University, Lubbock, TX 79409-1051, USA
[†] Physics Department, Washington University, St. Louis, MO 63130, USA
E-mail: `stefanke@zeus.phys.ttu.edu`

The interactions between hydrogen and intrinsic defects in silicon are systematically studied using *ab-initio* (tight-binding) molecular-dynamics simulations in supercells containing 64 and 216 host atoms and ab-initio Hartree-Fock calculations in clusters containing up to 100 Si atoms. The configurations, electronic structures, and binding energies of hydrogen bound to small vacancy aggregates are calculated. Both the vacancy and the self-interstitial efficiently dissociate interstitial H_2 molecules.[1] Vacancy-interstitial recombination at H_2 results in the formation of the H_2^* complex.[2] Ongoing research deals with the precipitation of H at defects. The very stable ring-hexavacancy,[3] an ellipsoidal void of diameter 7.8 Å and thickness 4.4 Å, is used as a model defect to study what happens when numerous H interstitials successively interact with such a defect. We also begun to study the interactions between self-interstitials, the formation of stable aggregates of $n = 2, 3, \ldots$ self-interstitials, and the trapping of H at such aggregates. This talk will begin with a summary of recently published results, continue with an overview of ongoing research, and conclude with a few speculation. Movies of molecular-dynamics simulations will be shown.

[1] S.K. Estreicher, J.L. Hastings, and P.A. Fedders, Phys. Rev. B **57**, R12663 (1998).
[2] S.K. Estreicher, J.L. Hastings, and P.A. Fedders, Phys. Rev. Lett. (in print).
[3] S.K. Estreicher, J.L. Hastings, and P.A. Fedders, Appl. Phys. Lett. **70**, 432 (1997).

SII.1: Interactions of hydrogen with silicon and consequences for devices

Chris G. Van de Walle

Xerox PARC, 3333 Coyote Hill Road, Palo Alto, CA 94304, USA
E-mail: `vandewalle@parc.xerox.com`

The recent resurgence of interest in the properties of hydrogen in semiconductors has been driven by a number of exciting developments: enhanced stability of defect passivation by using deuterium instead of hydrogen; hydrogen-induced exfoliation for producing silicon-on-insulator structures (the Smart-Cut$^{(R)}$ process); better control of hydrogen's influence on doping; and experimental observation of interstitial H_2 molecules.

A thorough understanding of the underlying mechanisms is essential for exploiting these processes. First-principles computations have significantly contributed to our body of knowledge about hydrogen-related phenomena; in this talk I will review our current understanding, and focus on recent work addressing the issues outlined above. The computational results have all been obtained using a state-of-the-art first-principles approach based on density-functional theory, *ab initio* pseudopotentials, and a supercell geometry. On the issue of stability of Si–H bonds, I will discuss the dissociation path and the connection to vibrational properties of the system; this immediately explains the enhanced stability of Si–D bonds. I will also discuss an exchange process between trapped and interstitial hydrogen that plays a significant role in diffusion processes. Relating to hydrogen-induced exfoliation, I will discuss current views on formation and structure of platelets. For hydrogen molecules, finally, I will describe the theoretical framework for understanding the physics of incorporation of a strongly bound molecule in a semiconducting environment.

I gratefully acknowledge collaborations with B. Tuttle, C. Herring, W. Jackson, N. Johnson, N. Nickel, and R. Street.

SII.2: Energy levels for muonium in silicon and germanium and electrical activity at high temperatures

S. F. J. Cox, R. L. Lichti[†], K. H. Chow[‡], E. A. Davis[§], T. L. Estle[♯], B. Hitti[♮], E. Mytilineou[§], C. Schwab[♭], A. Amato[¶], A. Schenck[◇], M. Charlton[*] and P. Donnely[*]

ISIS Facility, Rutherford Appleton Lab (OX11 0QX) and University College London
[†] Texas Tech University, USA, [‡] Lehigh University, USA, [§] Leicester University, Leicester, [♯] Rice University, [♮] TRIUMF, Canada, [§] Patras University, Greece, [♭] CNRS Strasbourg, France, [¶] Paul Scherrer Institute, Villigen-PSI, Switzerland, [◇] IPP ETH-Zurich, Villigen-PSI, Switzerland, [*] University College, London
E-mail: `SFJC@ISISE.RL.AC.UK`

Investigations of the transitions between the various sites and charge states of muonium in Si and Ge are described and the inferences for hydrogen considered.

The experiments use the μSR techniques of muon spin rotation, relaxation and resonance. These are capable of detecting the charged (diamagnetic) and neutral (paramagnetic) muonium states with equal sensitivity on a microsecond timescale, generally before reaction and pairing with other defects, dopants or impurities. State conversions are most readily recognised via relaxation (depolarization) in longitudinal magnetic field: one-way reactions, spin-exchange and two-way reactions involving capture and loss of carriers can all be distinguished. Field scans identify the active neutral centre by determining the intermittent hyperfine constant. Radiofrequency resonance is uniquely valuable in analysing for the final state in a reaction sequence. In high transverse magnetic field a paramagnetic shift of the muon Larmor precession signal is observed in charge-exchange regimes which indicates that muonium spends a surprisingly high fraction of its time in the neutral state above 600K, despite the rapidity of electron capture and loss.

A 4-state model (Mu^{+}_{BC}, Mu^{0}_{BC}, Mu^{0}_{T} and Mu^{-}_{T}) and corresponding configuration-coordinate diagram are consistent with the data and most theoretical input. Values for most of the relative energy levels and barriers, together with probabilities of site-change, ionization and carrier capture are available for Si. Preliminary values for Ge indicate that the potential energy surface for the neutral centres is much flatter than for Si, with the bond-centred (BC) and cage-centred (T) sites more nearly equal in energy than in Si and the barrier between them smaller. Both sites may be visited in the course of diffusion above 100K (contrary to Si, where only the T-site neutral is mobile); site changes without charge-state change remain slow at all temperatures in Ge so that the two single-site ionization energies may be measured separately. The BC site is the more stable by a small margin. The importance of both T and BC sites is also established in amorphous material.

The electrically active levels within the fundamental gap may be constructed from relevant level separations in the configuration coordinate diagram. (Since donor and acceptor levels involve energy differences, the isotope effects between muonium and hydrogen are expected to be relatively small.) The experiments are close to determining the site-change energies which are crucial to deciding whether muonium constitutes a negative-U centre in these materials.

SII.3: Effect of hydrogen on thermal double donor formation in silicon

L. Murin, V. P. Markevich, J. L. Lindström[†] and T. Hallberg[†]

Institute of Solid State and Semiconductor Physics Minsk 220072, Belarus
[†] Department of Physics and Measurement Technology Linkoping University Linkoping, Sweden
E-mail: `murin@ifttp.bas-net.by`

We start with an overview of the previously published data on the problem. The main unanswered questions are noted and discussed. We report also some new information on the peculiarities of the very early stages of oxygen clustering in hydrogenated Si. The data are obtained from the studies of the formation kinetics at 350–400 °C of small oxygen clusters (dimers, trimers and the first TDD species) in Czochralski-grown Si crystals pre-heat-treated at high temperature in the hydrogen gas. It is argued that hydrogen affects the migration ability not only of the interstitial oxygen atoms but of the small oxygen aggregates as well. With this in mind the possible TDD formation schemes are considered.

SIII.1: Hydrogen-defect complexes in silicon: Fact and speculation

B. Bech Nielsen

Institute of Physics and Astronomy, University of Aarhus, DK-8000 Aarhus C, Denmark
E-mail: `bbn@ifa.au.dk`

The atomic structure of the complexes formed when hydrogen becomes trapped by intrinsic defects in silicon can be investigated by structure sensitive techniques and *ab initio* theory. In particular, FTIR spectroscopy has been widely applied to study the local vibrational modes of hydrogen, which depend critically on the atomic structure of such complexes. From comparison of the observed modes with those calculated by *ab initio* theory, it has been possible to identify specific complexes in several cases. Moreover, valuable information about the electronic structure of a few hydrogen-defect complexes has recently been obtained by EPR, and a detailed picture has emerged from these correlated studies.

In this talk, an overview of our major findings on hydrogen-vacancy, hydrogen-interstitial, and hydrogen-impurity complexes will be presented and a few new results will be presented. At the end of the talk, it will be discussed how local mode frequencies may be assigned to specific structural units. On basis of this, tentative assignments will be suggested and their implications for diffusion and trapping of hydrogen will be briefly discussed.

SIII.2: Electrical properties of transition metal-hydrogen complexes in silicon

J. Weber

Max-Planck-Institut für Festkörperforschung, Postfach 80 06 65, D-70506 Stuttgart, Germany
E-mail: `weber@vaxff1.mpi-stuttgart.mpg.de`

Our recent studies on the properties of hydrogen in silicon doped with transition metals (TM) are summarized. In particular, we will concentrate on the substitutional TMs with their simple vacancy-like structure. Hydrogen was incorporated in the samples by wet chemical etching at room temperature or by hydrogen plasma treatment at elevated temperatures. Deep-level-transient spectroscopy (DLTS) on Schottky diodes reveals many new levels which are associated with transition metal-hydrogen complexes. The analysis of the deep level profiles gives valuable information about the number i of hydrogen atoms in the TM–H$_i$ complexes and in addition gives evidence for electrically passive complexes. All hydrogen related features disappear after heat treatments above 600 K for several hours. Systematic trends in the TM–H$_i$ level positions are discussed and compared to available experimental data and theory.

SIII.3: Defect profiles and the Feklisova–Yarykin conjecture

J. Coomer, A. Resende, R. Jones, S. Öberg [†] and P. R. Briddon [‡]

School of Physics, University of Exeter, Exeter EX4 4QL
[†] Department of Mathematics, University of Luleå, Luleå S95187, Sweden
[‡] Department of Physics, University of Newcastle upon Tyne, Newcastle upon Tyne NE1 7RU
E-mail: `coomer@excc.ex.ac.uk`
URL: `http://newton.ex.ac.uk/research/theory/jones/`

Deep level transient spectroscopy (DLTS) is a technique which allows the activation energies for the emission of carriers from deep levels to band edges to be measured. In many cases the energy level of the defect can then be extracted. However, a major drawback with the technique is that the chemical composition of the defect cannot be obtained and the types of atoms which make up the defect are then assumed to reflect the composition of the crystal. This of course does not provide any indication of the number of impurity atoms in the defect. This problem is particularly acute for H related defects where, for example, it is known from infrared absorption spectroscopy carried out on mixed H and D implanted material that vacancies in Si and Ge can be decorated from 1 to 4 H atoms. Feklisova and Yarykin have recently suggested a way in which mapping the concentration profile of the defect might yield its composition. They investigated the trapping of two defects created by electron irradiation, namely the VO defect (*A* centre) and a complex involving O and possibly C called the K centre. The former has a $(-/0)$ level at $E_c - 0.17$ eV and the latter acts as a hole trap with a level of unspecified character at $E_v + 0.33$ eV. This is close to the level for C_iO. H was introduced at room temperature using a wet chemical etch. New defects were then created and, in particular, E4 and E5 which are VO–H_n and C_iO_i–H_n defects respectively with levels at $E_c - 0.32$ and $E_c - 0.36$ eV. In addition, two unspecified hole traps H3, H4 lie at $E_v + 0.16$ and $E_v + 0.27$ eV. Now the profiles demonstrated that the concentrations of E4 and E5 behaved as $\mathrm{e}^{-2\mathrm{x}/\mathrm{L}}$ and $\mathrm{e}^{-\mathrm{x}/\mathrm{L}}$ respectively from which it was concluded that E4 was VOH_2 and E5 possesses only one H atom. With the above assignment this is then the C_iO_iH defect. However, the VOH_2 defect is expected to contain only saturated bonds and thus be inactive. This raises serious questions over the Feklisova and Yarykin analysis.

In order to investigate this, we have carried out first principles calculations with an empirical correction to ascertain the electrical levels of these defects. We find that the VOH_2 defect is inactive but VOH has a deep acceptor level.

We suggest that a better test of the Feklisova and Yarykin conjecture are depth profiles of V_2H_n defects with $n = 1, 2, 3, 4$ and 5. The structures and levels of these defects are reported.

SIII.4: Acceptor-like hydrogen dimers in silicon

B. Aradi and P. Deák

Technical University of Budapest, Department of Atomic Physics,
Budapest, Budafoki út 8, H-1111, Hungary
E-mail: `ab007@hszk.bme.hu`
URL: `http://qchem52.fat.bme.hu/index.html`

Recently it has been shown that luminescence at 1.151 and 1.138 eV in crystalline silicon is due to the recombination of excitons bound to isoelectronic acceptors containing two hydrogen atoms. Both centers are trigonal — in one of them the hydrogens are in equivalent positions, in the other one they are inequivalent. Both centers give rise to acceptor levels near the conduction band edge. The results of LDA-calculations on various hydrogen dimers will be presented to explain these observations.

SIV.1: Laplace transform DLTS studies of gold-hydrogen defects in silicon

A. R. Peaker, J. H. Evans-Freeman and L. Dobaczewski†

Centre for Electronic Materials, University of Manchester Institute of Science and Technology, PO Box 88, Manchester M60 1QD
† Institute of Physics, Polish Academy of Science, Al Lotnikow 32/46, Warsaw, Poland
E-mail: `peaker@umist.ac.uk`
WWW URL: `http://www.mcc.ac.uk/cem/`

We have used the technique of high resolution DLTS to study hydrogen-related complexes in silicon. Instead of using the rate window DLTS techniques pioneered by Lang, we have applied methods analogous to an inverse Laplace Transform to analyse carrier emission transients. In practice we use a form of Tikhonov regularisation (optimised for our experimental set up) to averaged isothermal carrier emission transients. With a signal to noise ratio of 1000:1 (in the averaged spectrum) we can routinely separate exponentials with a time constant ratio of 2:1. In practical terms this means we can achieve an order of magnitude improvement in resolution over conventional DLTS provided we have a suitable concentration of the defect (typically $0.1\,(N_d - N_a) > N_T > 0.01\,(N_d - N_a)$) and there are no other complicating factors (e.g. strong field dependence of the emission rate). This brings the technique into a regime where it is possible to quantify the effects, for example, of uniaxial stress or the local environment (e.g. in alloys) on carrier emission properties of a deep state.

Over the last year we have used the technique to examine the properties of gold-hydrogen defects in silicon. We have diffused gold into *n*- and *p*-type material and then introduced hydrogen by wet etching. The high resolution DLTS measurements have been carried out on Schottky diodes.

Our results at low hydrogen concentration are in good agreement with previous conventional DLTS studies, and furthermore, we are able to separate quite clearly the gold acceptor and

G4 and conclude from capture measurements that G4 is an acceptor. At higher hydrogen concentrations we see evidence of another state with electron emission characteristics close to G4 which we call G4′. From the dependence on hydrogen concentration it seems that this is AuH_2 assuming the previous assignment of G4 to the $-/0$ charge state of AuH to be correct. The state referred to as G1 which is believed to be the double acceptor $(=/-)$ of AuH shows no fine structure in high resolution DLTS, even at high hydrogen concentrations. We observe two additional defect signatures in n-type material in high hydrogen layers, which are quite undetectable at low hydrogen concentrations. These states are also in high hydrogen material that does not contain gold but the defect states appear to be present in lower concentrations. Work is currently in progress to try to identify these hydrogen-related deep levels.

In p-type material the situation is somewhat more complicated. Hole emission is observed from the state assigned G2 by previous workers which is thought to be the donor state of AuH $(0/+)$. From our high resolution DLTS measurements, G2 seems to exist in two configurations dependent on the hydrogen concentration and the history of the sample. We have undertaken uniaxial stress measurements on this centre and see splitting which we associate with a metastable reorientation of the defect under stress.

SIV.2: Electric field dependent structural and vibrational properties of the Si(100)-H(2×1) surface and its implications for STM induced hydrogen desorption

K. Stokbro

Mikroelektronik Centret (MIC), Technical University of Denmark, Building 345E,
DK-2800 Lyngby, Denmark
E-mail: `stokbro@loke.mic.dtu.dk`
URL: `http://www.mic.dtu.dk/mic/staff/ks.htm`

I will report a first principles study of the structure and the vibrational properties of the Si(100)–H(2×1) surface in an electric field. From the calculations one can extract parameters which can be used to model the vibrational modes in the presence of the electric field corresponding to a realistic STM tip-surface geometry. Such models show that local one-phonon excitations have short lifetimes (10 ps at room temperature) due to incoherent lateral diffusion, while diffusion of multi-phonon excitations are suppressed due to anharmonic frequency shifts and have much longer lifetimes (10 ns at room temperature). The implications for current induced desorption of H are calculated using a recently developed first principles model of electron inelastic scattering. The calculations show that inelastic scattering events with energy transfer $n\hbar\omega$, where $n > 1$, play an important role in the desorption process.

SIV.3: Hydrogen-passivation of double donors in silicon: atomic and electronic structure

P. T. Huy, C. A. J. Ammerlaan and T. Gregorkiewicz

Van der Waals-Zeeman Institute, University of Amsterdam, Valckenierstraat 65, NL-1018XE, Amsterdam, The Netherlands
E-mail: `pc-em01.wins.uva.nl`

Over the last ten years, the full passivation by hydrogen of shallow single donors and acceptors in silicon has been extensively investigated, both by experimental and theoretical methods as a result these passivated dopants have become well-understood defects. In some contrast, the understanding of the more complex and varied processes of passivation of deep electronic center is still not on a satisfactory level. The structure and corresponding electrical activity of hydrogen complexes with deep centers have proven to be intriguing results are controversial in several cases. The interactions of hydrogen with the chalcogen double donors are good examples of this situation. Experiments using deep level transient spectroscopy (DLTS),[1] infrared absorption[2] and magnetic resonance[3] showed that hydrogen can passivate the sulfur double donor in silicon. However, there still is dispute about the number of hydrogen atoms participating in the passivation process and about the question whether a single hydrogen complex will behave as a, possibly shallow, single donor. In our experiments the hydrogen passivation of the chalcogen double donors sulfur and selenium was studied. New results, to be reported, were obtained for selenium they will be put in perspective by comparing to the experimental[1−3] and theoretical[4] data available for the sulfur-hydrogen system. For selenium two new electron paramagnetic resonance (EPR) spectra, labeled Si-NL60 and Si-NL61, were observed. The spectra, both revealing trigonal symmetry, have been investigated in detail by ENDOR (electron-nuclear double resonance) and FSE (field-scanned ENDOR). By the use of both natural and isotopically enriched selenium (isotope ^{77}Se, nuclear spin $I = \frac{1}{2}$, natural abundance 7.6%, enriched 99.1%) the involvement of one selenium in the passivated centers was conclusively established. From the hyperfine structure due to hydrogen or deuterium, using heavy water with 99.95%, the presence of hydrogen was concluded. The Si-NL60 spectrum displays the nuclear interaction with one hydrogen atom. From the hyperfine and quadrupole interactions its is concluded that the corresponding center is very similar to the sulfur-hydrogen pairs (EPR spectra Si-NL54 and Si-NL55). The paramagnetic state most probably corresponds to the neutral charge state of a Si:SeH single donor. The other spectrum, Si-NL61, reveals hyperfine interaction with two inequivalent hydrogen atoms. For this Si:SeH2 center no corresponding sulfur-two-hydrogen pair was reported in preceding magnetic resonance experiments. The electronic and nuclear spin-Hamiltonian parameters of the Si-NL60 and Si-NL61 centers were determined by EPR and ENDOR. Models for atomic and electronic structure will be discussed on the basis of this information. Thermal annealing studies showed the centers to be stables up to temperatures around 600 °C. This result confirms the more stable bonding of hydrogen to double donors compared to the single ones. Measurements of annealing and conversion kinetics, applying uniaxial stress as well, are in progress.

[1] G. Pensl, G Roos, C. Holm, E. Sirtl and N. M. Johnson, Appl. Phys. Lett. 51, 451 (1987).

[2] R. E. Peale, K. Muro and A. J. Sievers, Mater. Sci. Forum **65-66**, 151 (1990).

[3] I. S. Zevenbergen, T. Gregorkiewicz and C. A. J. Ammerlaan, Phys. Rev. B **51**, 16746 (1995).

[4] V. J. B. Torres, S. Öberg and R. Jones, *Shallow-Level Centers in Semiconductors* (World Scientific, Singapore, 1997) p. 501.

SIV.4: Complexes of group-VI donors with hydrogen in GaP

B. Clerjaud, D. Côte and W. Ulrici[†]

Laboratoire d'Optique des Solides – UMR 7601, Université Pierre et Marie Curie,
case 80, F-75252 Paris cedex 05, France
[†] Paul-Drude-Institut für Festkörperelektronik, D-10117 Berlin, Germany
E-mail: `bec@ccr.jussieu.fr`

Photoluminescence measurements on sulfur-doped GaP performed before and after exposure to a radio frequency hydrogen plasma[1,2] suggested that hydrogen neutralizes group- VI donors in GaP. However, to our knowledge, group-VI donor-hydrogen complexes have not been directly evidenced until now in this material.

Sulfur, selenium and tellurium doped LEC grown GaP samples have been investigated by local vibrational mode (LVM) spectroscopy; as it is always the case for this type of material, hydrogen is also present in the samples with a concentration in the 10^{15}–10^{16} cm^{-3} range. LVM's at 2204, 2210 and 2217 cm^{-1} at 5 K are due to complexes of hydrogen with sulfur, selenium and tellurium respectively; sulfur doped deuterated samples have also been investigated and the LVM due to the sulfur-deuterium complex is at 1617 cm^{-1}. These wave numbers indicate that hydrogen binds one of the host phosphorus atoms which are next nearest neighbors of the group-VI donor. It has to be noted that no bending modes of the complexes could be observed.

Experiments under uniaxial stress have been performed. Their results cannot be interpreted in the frame of the conventional models.[3,4] A new model has been developed. It shows that the complexes have C_s symmetry and that the symmetry planes of the complexes are (110) and equivalent planes. The precise orientation of the induced electric dipole moment of the LVM in this plane is determined for each complex. The P–H bond is not along one of the main crystallographic axes as it is usually the case for hydrogen-shallow dopant complexes. A complete microscopic description of the complexes is given.

It comes out that the group-VI donor-hydrogen complexes in GaP are completely different from those observed in GaAs and AlSb where hydrogen binds one of the host group-III atoms nearest neighbors to the donor.

[1] J. Weber and M. Singh, Mat. Res. Soc. Symp. Proc. **104**, 325 (1988).

[2] M. Singh and J. Weber, Appl. Phys. Lett. **54**, 424 (1989).

[3] A. A. Kaplianskií, Opt. Spektrosc. **16**, 602 (1964); Opt. Spectrosc. **16**, 329 (1964).

[4] A. E. Hughes and W. A. Runciman, Proc. Phys. Soc. London **90**, 827 (1967).

Posters

P1: Hydrogenation of electron irradiation damage in silicon

J. H. Evans-Freeman and A. R. Peaker

Centre for Electronic Materials, University of Manchester Institute of Science and Technology, PO Box 88, Manchester, M60 1QD
E-mail: `j.evans-freeman@umist.ac.uk`
URL: `http://www.mcc.ac.uk/cem/`

Using high resolution Laplace DLTS, we have measured the electron emission characteristics of the di-vacancy and related defects in electron irradiated silicon. The irradiation was with 2 MeV electrons. A comparison has been made before and after room temperature diffusion of atomic hydrogen from the surface, which was introduced by wet chemical etching.

We identify the reaction products of hydrogen and the A centre as an electron trap with an activation energy of ~ 0.31 eV and in addition one or more inert species. By comparison with *ab initio* calculations we also assign Laplace DLTS features to the reaction products of the divacancy and hydrogen. These defects are very close in emission characteristics to the states previously assigned to the divacancy, but can be clearly separated using the Laplace technique.

P2: Hydrogen interaction with dislocation solitons in Si

S. Leoni, C. P. Ewels and M. I. Heggie

CPES, University of Sussex, Falmer, Brighton
E-mail: `ewels@charles.mols.susx.ac.uk`
WWW URL: `http://tc.cpes.susx.ac.uk/`

It is well known that hydrogen interacts with dislocations in silicon. For example, dislocation velocity in the presence of hydrogen plasma is enhanced with the barrier to motion dropping from 2.2 eV to 1.2 eV.[1] However the nature of these interactions are not well understood.

Dislocation motion can proceed either through reconstructed kink formation and migration, through the formation and propagation of reconstruction defects ("solitons"), or a combination of the two. It has been proposed that solitons are responsible for, amongst other things, kink relaxation dynamics.[2] Therefore a thorough understanding of the behaviour of solitons is crucial to understanding the mechanisms of dislocation motion.

In order to understand the interaction between hydrogen and solitons, we examine several possible bonding configurations between the two. We find that hydrogen can bond strongly to isolated solitons. We determine the vibrational characteristics of such hydrogen-soliton centres, and discuss the implications of soliton-hydrogen interactions for dislocation motion.

[1] Y. Yamashita, F. Jyobe, Y. Kamiura, K. Maeda, Phys. Stat. Solidi A **171**, 27 (1999).
[2] M. I. Heggie and R. Jones, Phil. Mag. B **48**, 365 (1983); **48**, 379 (1983).

P3: Donor formation in germanium by hydrogen plasma treatment

V. V. Litvinov, N. M. Kazuchitz, A. A. Klechko and A. G. Ulyashin [†]

Belarussian State University, Minsk 220050, Belarus
[†] Belarussian State Polytechnical Academy, Minsk 220027, Belarus
E-mail: `litvvv@phys.bsu.unibel.by`

A spreading resistance probe analysis of hydrogen-plasma-treated Ge crystals with different concentrations of shallow dopants and oxygen is presented. The samples were treated in dc H-plasma at 260, 300 and 350 °C for 0.5 and 1.5 hours. An enhanced formation of donor centers was observed in all the treated samples. The appearance of p-n junctions was revealed in p-type Ge.

The formation of O–H complexes and oxygen-related thermal donors is suggested to occur in Ge:O crystals under H-plasma treatment.

P4: Shallow donor centers in hydrogenated Cz-Si crystals

V. P. Markevich, L. I. Murin, T. Mchedlidze, M. Suezawa[†] and J. L. Lindström[‡]

Institute of Solid State and Semiconductor Physics, Minsk 220072, Belarus
[†] Institute for Materials Research, Tohoku University, Sendai, Japan
[‡] Department of Physics and Measurement Technology, Linkoping University, Linkoping, Sweden
E-mail: `murin@ifttp.bas-net.by`

The results of EPR and infrared absorption studies of shallow donor centers which are introduced into hydrogenated Cz-Si crystals as a result of electron irradiation and/or heat-treatments in the temperature range of 300–500 °C are reported. It is shown that the same shallow donor species are generated in both the pre-irradiated and non-irradiated Cz-Si:H crystals during heat-treatments at about 470 °C. Preliminary irradiation was found to result in enhanced formation of the donors. The possible atomic structures and formation mechanisms of the shallow donors in hydrogenated Cz-Si crystals are discussed.

P5: Muonium as a hydrogen analogue in silicon and germanium; quantum effects and hyperfine parameters

A. R. Porter, M. D. Towler and R. J. Needs

TCM Group, Cavendish Laboratory, Madingley Road, Cambridge, CB3 0HE
E-mail: `arp28@phy.cam.ac.uk`
URL: `http://www.tcm.phy.cam.ac.uk/~arp28/`

We present an all–electron theoretical study of muonium and hydrogen impurities in silicon and germanium. The electron–electron interactions are described within density functional theory

using the local density approximation and a generalized gradient approximation. A double adiabatic approximation is employed and we minimize the energy of muonium or hydrogen at the bond–centred site with respect to all degrees of freedom. At this level of approximation the relaxations of the host atoms are different for the muon and proton. The extra relaxations of the silicon and germanium atoms due to the zero–point motion of a muon at the bond centred site are quite small, while those for the proton are even smaller. The zero–point energy for a muon at the bond centred site is considerably larger than at the tetrahedral site. When zero–point motion is included the muon is more stable at the tetrahedral site than at the bond–centre. The hyperfine and superhyperfine parameters are calculated as averages over the motion of the muon, and are compared with previous calculations and with experiment.

P6: Ab initio simulation of hydrogen in silicon

M. I. J. Probert and M. C. Payne

TCM Group, Cavendish Laboratory, Madingley Road, Cambridge, CB3 0HE
E-mail: `mijp2@phy.cam.ac.uk`
URL: `http://www.tcm.phy.cam.ac.uk/~mijp2`

We present the results of ab initio path integral molecular dynamics calculations of hydrogen in silicon. The technique used is based on the Feynman path integral formulation of quantum mechanics, which is used to treat the atomic nucleus as a quantum object. Standard DFT techniques are used to treat the electrons in an ab initio fashion. This combined approach enables us to properly treat quantum fluctuations such as tunneling and zero point motion of the hydrogen atom.

The detailed properties of hydrogen are often probed experimentally by the muSR technique. Although muonium is chemically identical to hydrogen, it has a smaller mass and may therefore be substantially affected by quantum nuclear fluctuations, such as zero point motion and tunneling. There is therefore a need to simulate the properties of both hydrogen and muonium in silicon and test the effect of such fluctuations. Similar calculations for muonium are underway.

The results that we present show that these nuclear quantum fluctuations can make a significant difference to the energetics and structures formed. This therefore has important implications for the interpretation of experimental results and our basic understanding of the properties of hydrogen-like atoms in silicon.

P7: A novel vacancy-related muon species in crystalline silicon

M. Schefzik[†], R. Scheuermann[‡*], L. Schimmele[‡], A. Seeger[†‡], O. Kormann[‡], J. Major[†‡] and A. Röck[†]

[†] Universität Stuttgart, Institut für Theoretische und Angewandte Physik, Pfaffenwaldring 57, D-70569 Stuttgart, Germany
[‡] Max-Planck-Institut für Metallforschung, Heisenbergstr. 1, D-70569 Stuttgart, Ger-

many E-mail: `schefzik@physix.mpi-stuttgart.mpg.de`
* Present address: Muon Science Laboratory RIKEN, Wako, Japan

The positive muon (μ^+) can be considered as light isotope of hydrogen from the viewpoint of solid-state physics. It is an ideal tool for the study of isolated centres in semiconductors which are analogous to hydrogen centres. Low-temperature investigations of positive muons (μ^+) in crystalline silicon by means of two different techniques provide us with evidence of a novel paramagnetic muon species with weak, anisotropic hyperfine interaction (Solid State Comm. **107**, 395 (1998)). It adds to the list of known muon species, i.e. normal (tetrahedral position, $\mathrm{Mu_T}$) and anomalous (bond-centered position, $\mathrm{Mu_{BC}}$, analogous to the AA9 hydrogen centre) muonium and the diamagnetic muon species. The signatures of the novel species $\mathrm{Mu_V}$ are found in intrinsic but not in doped samples (dopant concentration about 10^{16} cm^{-3}). Longitudinal field quenching experiments reveal that $\mathrm{Mu_V}$ is not formed promptly. It results from a reaction in which normal muonium transforms into $\mathrm{Mu_V}$, the reaction rate at $T = 10$ K was found to be about 10^6 s^{-1}. The hyperfine coupling of $\mathrm{Mu_V}$ is determined from zero-field muon spin precession experiments. The hyperfine tensor is found to be axially symmetric with the components $A_\mathrm{x} = A_\mathrm{y} = -12.0$ MHz and $A_\mathrm{z} = 28.75$ MHz, with the z axis pointing into the $\langle 110\rangle$ crystallographic direction. It corresponds, after rescaling, to the hyperfine tensor of the hydrogen centre termed VH, which was discovered recently by Bech Nielsen *et al.* (Phys. Rev. Lett. **79**, 1507 (1997)) and which has been attributed to hydrogen trapped in vacancies. This novel muon species $\mathrm{Mu_V}$ is tentatively interpreted as muonium trapped in vacancies, which are created during deceleration of the implanted muon close to the end of its stopping track.

The authors are indebted to Dr. W. Zulehner, Wacker Siltronic AG, Burghausen, Germany for kindly providing the samples. The support of the directorate and the technical staff of the Paul Scherrer Institut is gratefully acknowledged. This work was funded by the Bundesministerium für Bildung und Forschung, Bonn, Germany under contract Nos. 03-MA5ST1 and 03-MA5ST2.

P8: Neutral fraction of muonium and hydrogen in silicon at elevated temperatures

S. F. J. Cox, A. Amato [†], A. Schenck [‡], M. Charlton [§] and P. Donnelly [§]

Rutherford Appleton Laboratory, Chilton, Oxfordshire OX11 OQX
† Paul Scherrer Institute, Villigen-PSI, Switzerland
‡ IPP ETH-Zurich, Villigen-PSI, Switzerland
§ University College, London
E-mail: `SFJC@ISISE.RL.AC.UK`

Measurements of a paramagnetic shift of the muon Larmor frequency in silicon indicate that muonium — and by inference hydrogen — defect centres spend a surprisingly high proportion of their time in the neutral charge state above 600 K, despite the rapidity of electron loss (ionization) and recapture. The data should allow determination of the relevant electrically active energy level.

P9: High field EPR & ENDOR measurements on V_nH complexes in silicon

R. J. Dirksen, M. S. Visser, T. Gregorkiewicz and C. A. J. Ammerlaan

Van der Waals-Zeeman Institute, University of Amsterdam, Valckenierstraat 65, NL-1018XE, Amsterdam, The Netherlands
E-mail: `dirksen@phys.uva.nl`

Proton irradiated silicon samples have been studied with magnetic resonance. The EPR experiments have been conducted at X, K, and D microwave bands of 9, 23, and 140 GHz, respectively.

Hyperfine interactions have been carefully followed by ENDOR. The measurements were performed at different temperatures and microwave power levels.

The obtained spectra and their angular dependences are compared with simulations based on the existing models of V_nH centers (VH, V_2H, V_3H).

P10: Hydrogen-related complexes in SiC

A. Gali, J. Miro and P. Deák

Technical University of Budapest, Department of Atomic Physics,
Budapest, Budafoki út 8, H-1111, Hungary
E-mail: `ga043@hszk.bme.hu`
URL: `http://qchem52.fat.bme.hu/index.html`

Hydrogen is the main impurity in silicon carbide (especially in CVD-grown layers) which is the most promising semiconductor at present for high power/temperature/frequency applications. *Ab initio* LDA calculations have been used to study hydrogen related defects in intrinsic SiC. Relative stabilities, occupation levels and vibrational modes have been calculated and compared to existing experimental data. Interesting differences with respect to H in Si have been found.

P11: A muon study of Czochralski silicon at high temperatures

P. King

ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon, OX11 0QX
E-mail: `philip.king@rl.ac.uk`
URL: `http://www.isis.rl.ac.uk/muons/`

Czochralski silicon contains high levels of oxygen, which, during anneals between 570–820 K, forms thermal donor complexes. Complex formation is enhanced by the presence of hydrogen which is believed to catalyse the oxygen diffusion, although the precise mechanism for this is still a matter of investigation.

Much of our knowledge of isolated hydrogen behaviour in silicon has come from studies of the behaviour of its light isotope muonium, formed by implanting spin polarised positive muons.

Above room temperature, the muon polarisation decay follows a simple exponential, and this is believed to be due to a charge exchange (CE) reaction involving repeated ionisation of muonium followed by electron capture.

In this study we present results from muon investigations of Czochralski silicon at high temperatures. A sample heat treated to precipitate the oxygen shows very similar behaviour to float zone material when the CE model is applied; the CE model seems to describe untreated material much less satisfactorily, and this is attributed to the presence of oxygen. Observation of the muon behaviour in this latter case provides information on the nature of the muon species involved and may help elucidate the role of hydrogen in oxygen diffusion.

P12: Local vibrational mode bands of V-O-H complexes in silicon

V. P. Markevich, L. I. Murin, J. L. Lindström[†] and M. Suezawa[†]

Institute of Solid State and Semiconductor Physics, Minsk 220072, Belarus
[†] Department of Physics and Measurement Technology, Linkoping University, Linkoping, Sweden
[‡] Institute for Materials Research, Tohoku University, Sendai, Japan
E-mail: `murin@ifttp.bas-net.by`

Infrared absorption study of formation and annealing of radiation-induced defects in hydrogenated Czochralski-grown silicon crystals have been performed. Hydrogen and/or deuterium was introduced into the crystals by in-diffusion from H_2 (D_2) gas at 1200–1300 °C. The samples were irradiated with fast electrons (E = 2-4 MeV) and annealed in the temperature range of 100–600 °C. The dominant centres produced by irradiation were found to be the same in both Si:O,H and as-grown materials: *A* centre, C_i-O_i complex and divacancy. A profound effect of hydrogen was revealed in the annealing behaviour of radiation-induced defects. The disappearance of them in hydrogenated crystals occurred at lower temperatures beginning from 100 °C and was followed by a creation of a number of new infrared absorption bands in wavenumber regions characteristic for the oxygen- and hydrogen-related local vibrational modes (LVMs) in silicon. Disappearance of A centres in the temperature range of 100–150 °C was found to correlate with the appearance of three LVM bands at 943.5, 2126.4 and 2151.5 cm^{-1}. Substitution of hydrogen by deuterium resulted in a shift of the lines to 943.2, 1549.1 and 1567.4 cm^{-1}. In the samples co-doped with H and D in addition to these lines two other ones were observed at 1557.3 and 2140.6 cm^{-1}. It was suggested that the lines are related to LVMs of a complex V-O-H_2. The complexes are formed by the interaction of mobile hydrogen molecules with the A centres. The V-O-H_2 complex is stable up to 200 °C. Simultaneously with the disappearance of the LVM bands due to V-O-H_2 complex at higher temperatures an absorption band at 891.5 cm^{-1} was developed. A line at the same position was observed in deuterated samples. No correlation was found between the appearance of this band and the development of any bands in the range which is characteristic for stretching vibrations of hydrogen (deuterium) atoms in Si. The line at 891.5 cm^{-1} is preliminary identified as related to the stretching vibrations of oxygen atoms in a complex VO_2 with a hydrogen molecule in the vicinity.

P13: Vibrational modes of VOH_2 in Si

J. Coutinho, A. Resende, R. Jones, S. Öberg [†] and P. R. Briddon [‡]

School of Physics, University of Exeter, Exeter EX4 4QL
[†] Department of Mathematics, University of Luleå, Luleå S95187, Sweden
[‡] Department of Physics, University of Newcastle upon Tyne, Newcastle upon Tyne NE1 7RU
E-mail: `coutinho@excc.ex.ac.uk`
URL: `http://newton.ex.ac.uk/~coutinho/`

The structure and vibrational modes of VO–H_2 defect in Si are calculated using a first principles cluster method (AIMPRO). The calculated modes are compared with those reported by Markevich *et al.* at this conference.

P14: The electrical properties of transition metal hydrogen complexes in silicon: A theoretical study

A. Resende, R. Jones, S. Öberg [†] and P. R. Briddon [‡]

School of Physics, University of Exeter, Exeter EX4 4QL
[†] Department of Mathematics, University of Luleå, Luleå S95187, Sweden
[‡] Department of Physics, University of Newcastle upon Tyne, Newcastle upon Tyne NE1 7RU
E-mail: `resende@excc.ex.ac.uk`
URL: `http://newton.ex.ac.uk/~resende/`

The electrical levels of various combinations of transition metal–H_n defects in Si are calculated and compared with recent transient capacitance measurements. Spin-polarised local density functional cluster theory is used. The shifts of these levels with H can be understood through a displacement and splitting of the gap t_2 manifold of states due to the impurity. Passive defects are identified. The similarities between Au– and Ag–H defects, and Pt– and Pd–H defects are discussed.

P15: Theoretical investigation of the structural, vibrational and electrical properties of multi-hydrogen vacancy defects in silicon

A. Resende, J. P. Goss, R. Jones, S. Öberg [†] and P. R. Briddon [‡]

School of Physics, University of Exeter, Exeter EX4 4QL
[†] Department of Mathematics, University of Luleå, Luleå S95187, Sweden
[‡] Department of Physics, University of Newcastle upon Tyne, Newcastle upon Tyne NE1 7RU
E-mail: `resende@excc.ex.ac.uk`
URL: `http://newton.ex.ac.uk/~resende/`

Large H-terminated clusters ($Si_{181}H_{116+n}$) are used to simulate the properties of VH_n defects with $n = 1$ to 4 within the framework of the local spin density functional theory.

Our calculations have shown that for VH_1 and VH_2, the reconstructed bond across two Si neigbours of the vacancy plays an important role on the their vibrational and electrical properties.

The H-stretch mode frequencies are calculated within an error bar of 0.1–0.5% relatively to the observed ones. The vibrational properties of VH_3 are compared with those of V_2H_6, together with recent electron paramagnetic resonance and Fourier transform infra-red spectroscopic studies.

5.2 Reports on Collaborative Visits

Report on a visit of C. Filippi (University College Cork, Ireland) to Prof. Scheffler's group (Fritz-Haber Institute, Berlin)

February 23-27

My visit to Prof. Scheffler, Dr. Kratzer and Dr. Pehlke at the Fritz-Haber Institute in Berlin was very important in order to be able to set up our collaboration. Our long-term goal is to perform a computational study of the adsorption/desorption mechanism of molecular hydrogen on Si(100) surface using quantum Monte Carlo (QMC) techniques.

The interaction of hydrogen with the silicon surface poses several interesting problems. The desorption of H_2 from Si(100) follows first-order kinetics, posing definite constraints on the possible desorption mechanism. The sticking coefficient of hydrogen on silicon is very small, indicating a high barrier to adsorption, while no substantial adsorption barrier has been observed in desorption experiments. Theoretically, various desorption mechanisms have been proposed to explain these experimental findings. Density functional theory calculations by Scheffler, Kratzer and Pehlke on extended slab geometries promote a "pre-pairing" mechanism of the hydrogens before desorption, find an agreement with experiments on the desorption barrier height and are able to explain the small sticking coefficient of hydrogen on silicon. However, they disagree with experiments on the height of the adsorption barrier. Moreover, quantum chemistry calculations on model clusters lead to a completely different mechanism of desorption.

During my short visit, we established how to approach the problem in the most effective way taking into consideration the technical limitations of QMC calculations. The project will take several months and we expect to have a few publications as a result of this work.

Claudia Filippi

5.3 Workshop Announcements

5.3.1 Workshop on Computational Materials Science

Dipartimento di Fisica, Universita‘ di Cagliari Istituto Nazionale per la Fisica della Materia,
Unita‘ di Cagliari

IX WORKSHOP ON COMPUTATIONAL MATERIALS SCIENCE
10 - 13 September 1999
Tanka Village, Villasimius (CA)
web page: **http://www.dsf.unica.it/CMS99**
under the patronage of UNESCO
with the sponsorship of ESF Psi-k Programme, Regione Autonoma Sardegna, Comune di Villasimius, Agrosarda

See PROGRAM and REGISTRATION INFO below.

FORMAT: About 20 invited lectures plus POSTER contributed session.

VENUE: Tanka Village at Villasimius (CA), an attractive sea resort on the south-eastern coast of Sardinia, providing comforts and an informal atmosphere.

CONTACT: For scientific queries:
vincenzo.fiorentini@dsf.unica.it
paolo.ruggerone@dsf.unica.it

For logistics: Corsi&Congressi, Cagliari, corsieco@tin.it

CONTRIBUTIONS AND PROCEEDINGS:
Contributions in poster format are invited. ALL contributions will be probably published in a special issue of the journal Computational Materials Science. Deadline for abstract submission: July 31, 1999. Contact V. Fiorentini at +39 070 6754912 or P. Ruggerone at +39 070 6754847 or at vincenzo.fiorentini@dsf.unica.it or paolo.ruggerone@dsf.unica.it for further details. Manuscripts will be due at the Workshop.

FRIDAY SEPTEMBER 10

Morning: working session 1: THEORY OF MATERIALS: DENSITY FUNCTIONAL AND BEYOND

8.30	E. K. U. Gross (Universitaet Wuerzburg)
9.30	R. Resta (Universita‘ di Trieste)
11.00	R. Godby (University of York)

Afternoon: working session 2: SOFT AND GRANULAR MATTER

17.30 V. Marinari (Universita‘ di Cagliari)
18.30 D. Wolf (Universitaet Duisburg)

SATURDAY SEPTEMBER 11

Morning: working session 3: ORGANIC AND BIO-SYSTEMS

08.30 C. Molteni (Cavendish Lab., Cambridge)
09.30 B. Smit (Amsterdam Universitet)
11.00 F. Seno (Universitá di Padova)

Afternoon: working session 4: SOLID-STATE APPLICATIONS

17.30 J. Kohanoff (Abdus Salam Center for Theoretical Physics, Trieste)
18.30 R. Godby (University of York)

SUNDAY SEPTEMBER 12

Morning: working session 5: GROWTH AND REACTIVITY

8.30 D. Wolf (Universitaet Duisburg)
9.30 B. Smit (Amsterdam Universitet)

Afternoon: excursion

21.00 Poster session with refreshments

MONDAY SEPTEMBER 13

Morning: working session 6: NEW COMPUTATIONAL METHODS

8.30 R. Resta (Universita‘ di Trieste)
9.30 J. Kohanoff (Abdus Salam Center for Theoretical Physics, Trieste)
11.00 S. Baroni (International School for Advanced Studies, Trieste)

Afternoon: working session 7: THEORY AND PRACTICE OF NANOSTRUCTURES: A PERSPECTIVE

17.30 E. Molinari (Universita‘ di Modena)
18.30 R. Cingolani (Universita‘ di Lecce)

REGISTRATION

Please send the REGISTRATION form by fax or e-mail, STRICLY before July 1, 1999 to

Corsi&Congressi
via Ghibli 8, I-09126 Cagliari
tel +39 070 383373
fax +39 070 3837102
e-mail: corsieco@tin.it

The registration MUST BE ACCOMPANIED BY PAYMENT RECEIPT OF THE CONFERENCE FEE. The fee includes full-board lodging at Tanka Village from 9/9 dinner to 14/9 breakfast, coffee breaks, and excursion, and it amounts to:

Double room lodging: Italian Lire 850000 (~US $475)/person
Single room lodging: Italian Lire 950000 (~US $535)/person

PAYMENT should be effected by bank money transfer on the bank account # 27660 of Corsi&Congressi, at Credito Italiano, via Scirocco 46/A, 09126 Cagliari, Codice ABI 02008 - CAB 04804.

No fee is requested from the invited speakers.

The Organizing Committee hopes to be able to offer partial support to a limited number of young scientists, preferrably PhD students. Since this possibility depends on funds availability, support will be decided upon only shortly before the workshop.

REGISTRATION FORM

Name ....
Institution ....
e-mail address ....
Arrival date: / /99 - Departure date: / /99
Accomodation: Single room [_] Double room [_]
Plan to present a poster entitled:

Series Chairman : prof. A. Baldereschi - EPFL Lausanne
Workshop Chairman : prof. F. Meloni - INFM and Universita‘ di Cagliari
Scientific Secretariat: dr. V. Fiorentini - dr. P. Ruggerone
INFM and Universita‘ di Cagliari

6 General Workshop/Conference Announcements

6.1 CECAM Tutorial

CECAM tutorial: 3 days on molecular dynamics and path integrals

Mark E. Tuckerman
Department of Chemistry and Courant Institute for Mathematical Sciences
New York University, New York, NY 10003
Glenn J. Martyna
Department of Chemistry, Indiana University, Bloomington, IN 47405–4001

Abstract

This workshop is designed to give participants a detailed introduction to path integrals and their use in computational chemistry and to the evaluation of path integrals by molecular dynamics techniques. The first day of the workshop will be devoted to providing the background in modern molecular dynamics theory and methodology necessary to understand how it is applied to the path integral. Thus, multiple time scale integration techniques, non-Hamiltonian statistical mechanical theory and its implications for molecular dynamics, and integration algorithms for non-Hamiltonian systems are among the topics that will be covered. The second day of the workshop will focus on the path integral as a computational approach to quantum statistical mechanical problems in chemistry and chemical physics. The derivation of the path integral will be discussed, including how to obtain thermodynamic quantities and expectation values of operators from the path integral. The molecular dynamics approach to path integrals will be described in detail, incorporating topics covered on the first day. A number of recent applications of the path integral to fundamental problems in chemistry will be presented. The third day of the workshop will be devoted to more advanced path integral techniques, which may include the centroid dynamics approach to approximate quantum dynamical properties, path integrals at constant pressure, *ab initio* path integrals and parallelization strategies for path integral molecular dynamics. Each day of the workshop will encompass three approximately 1-hour lectures in the morning following by hands-on computer exercises in the afternoon.

Monday

Morning:

I. Lecture I: Hamiltonian molecular dynamics and multiple time scale integration.

  - Hamilton's equations, phase space, and phase space evolution.
  - The Liouville operator and the classical propagator.
  - The Trotter theorem, factorization of the propagator, simple integrators and the direct translation technique.
  - Multiple time scale (MTS) factorizations and MTS integrators.
  - Examples.

II. Lecture II: Statistical theory of non-Hamiltonian systems its relation to molecular dynamics.

  - Non-Hamiltonian phase spaces and invariant measures.
  - The non-Hamiltonian Liouville equation.
  - Conservation laws and the microcanonical partition function of a non-Hamiltonian system.
  - Designing non-Hamiltonian molecular dynamics algorithms.
    i. The canonical (NVT) ensemble.
    ii. The isothermal-isobaric (NPT) ensemble.
    iii. The isothermal constant surface-tension ($N\sigma T$) ensemble.

III. Lecture III: Integrators for non-Hamiltonian systems.

- Why the operator-based approach is needed.
- Factorizing a non-Hamiltonian classical propagator.
- The Suzuki-Yoshida decomposition in general.
- The Suzuki-Yoshida decomposition for the (NVT) and (NPT) ensembles.
- Multiple time scale integrators for non-Hamiltonian systems.
- Examples.

Afternoon:

I. Computer exercises

Tuesday

Morning:

I. Lecture I: Quantum statistical mechanics and the path integral.

  - The quantum mechanical density matrix.
  - Derivation of the discrete path integral.
  - The functional integral form.

  - Thermodynamics from the path integral.
  - Expectation values of operators.

II . Lecture II: Molecular dynamics evaluation of the path integral.

  - Molecular dynamics vs. Monte Carlo.
  - Difficulties of path integral MD.
  - Staging and normal mode transformations.
  - A path integral molecular dynamics Hamiltonian.
  - Thermostatted equations of motion and multiple time scale integration.
  - Tests and comparisons with Monte Carlo.

III . Lecture III: Applications of path integral molecular dynamics.

  - Proton transfer in acidic and basic aqueous clusters.
  - Proton transfer in acidic solutions.
  - Intramolecular proton transfer.
  - Quantum effects in alkanes.
  - Para-hydrogen and ortho-deuterium.
  - Liquid ammonia.

Afternoon:

I. Computer exercises

Wednesday

Morning:

I. Lecture I: Centroid molecular dynamics.

  - The centroid distribution function.
  - Quantum time correlation functions and centroid time correlation functions.
  - Classical theory of adiabatic dynamics.
  - Adiabatic centroid molecular dynamics.

  - Examples.

II. Lecture II: Constant pressure path integral molecular dynamics.
  - The quantum NPT ensemble.
  - Pressure estimators.
  - Virial theorems and centroid virial theorems.
  - Full and reduced molecular dynamics algorithms.
  - Example applications.

II. (Alternative) Lecture II: Ab initio path integrals.
  - Density functional theory and the basics of ab initio molecular dynamics.
  - The path integral Born-Oppenheimer approximation.
  - Car-Parrinello ab initio path integral molecular dynamics.
  - Examples.

III. Lecture III: Parallel implementation of path integral molecular dynamics.
  - Implementation of bead-level parallelization.
  - Communicators, groups and dual-level parallelization.
  - Dual-level parallelization of path integrals.
  - Examples of timings.

Afternoon:

I. Computer exercises

6.2 2^{nd} Circular ECDM-II and call for Abstracts

Second European Charge Density Meeting

ECDM-II website

For all update information about the conference and registration, please see our website:

http://www.icmab.es/ecdmii.

Venue, location and accommodation

The 2nd European Charge Density Meeting will be held at the Calpolis Hotel (****) in Sitges (Barcelona). Sitges is a warm village located on the coast at about 35 Km South of Barcelona and can be easily reached by car or train. Barcelona is served by the El Prat International Airport (20 km from Sitges).

Accommodation at moderated rates is arranged at the Calpolis Hotel (****), where ECDM-II will take place (see "Registration fee").

Tourism information about Sitges can be obtained at: http://www.sitgestur.com Tourism information about Barcelona can be obtained at: http://www.bcn.es

Abstracts submission

We strongly recommend the submission of abstracts via e-mail to the address: **ecdmii@icmab.es**.

Please, write the related session of your contribution (A, B, C or other: see "Scientific Programme") in the subject field of your e-mail.

Please attach your abstract document (preferably in MS Word) to your e-mail.

Aside from the abstract, your e-mail should contain the following information:

Family name:
First name:
Title:
Department:
Institution:
Street:
City:
Zip/Post Code:
Country:
E-mail:
Fax:

Abstract title:
Related session (A, B, C, other: see "Scientific Programme"):
I wish to present a (poster, oral communication*):

* The Scientific Committee will choose the oral communications among the received abstracts. Oral communications are intended of about 20 minutes.

Abstract submission instructions (see example below)

The entire abstract, including title, authors and their affiliations, footnotes, references, diagrams, tables, equations, etc., must fit into a rectangle 12 cm wide by 17 cm high. We recommend the submission of abstracts in Times font, 10 point size, single line spaced. Use the symbol font for special characters, such as Greek letters. The title should be in UPPER CASE letters in bold and authors names in italic (the presenting author underlined). A blank line should be left between title and authors, between authors and the abstract main body and between this one and references.

Example:

THE HYDROGEN BOND STRENGTH IN TERMS OF THE TOPOLOGICAL PROPERTIES OF THE ELECTRON DENSITY DISTRIBUTION.

E. Espinosa[1,2], *E. Molins*[1] *and C. Lecomte*[2]

[1]Institut de Cincia de Materials de Barcelona (CSIC). Campus de la UAB, 08193 Cerdanyola (Barcelona), Spain. [2]Laboratoire de Cristallographie et Modlisation des Matriaux Minreaux et Biologiques, UPRESA CNRS 7036, Universit Henri Poincar, Nancy 1, BP 239, 54506 Vandoeuvre-ls-Nancy CEDEX, France. E-mail: enrique@icmab.es

Interatomic interactions such as hydrogen bonds (HBs) can be adequately described and classified by the topological properties of the electron density ?(r) at the (3,-1) critical points rCP, where the gradients of ?(r) vanish [1]. We have analysed [2] the topological properties of ?(r) at the intermolecular critical points of 83 experimentally observed HBs [X-H...O (X= C, N, O)] on a large set of compounds, obtained from accurate X-ray diffraction experiments. In spite of different models, methods and experimental conditions employed to obtain the topological properties of ?(r), we show that, for closed-shell interactions, the kinetic energy density G(rCP) and the potential energy density V(rCP) at the critical point, depend exponentially on the H...O distance [3]. We point out the positive correlation found between the V(rCP) and the HB energy when their functionalities against the H...O distance are compared. Recently [4], we have also observed that the positive and the negative curvatures of ?(r) at the H...O critical point exhibit linear relationships against, respectively, G(rCP) and V(rCP). The proportional behaviours found between those quantities show that the strength of the hydrogen bond interaction can be indistinctly interpreted in terms of any of them.

1.- R.F.W. Bader Atoms in Molecules: a Quantum Theory (Clarendon Press, Oxford, 1990). 2.- E. Espinosa, M. Souhassou, H. Lachekar and C. Lecomte. Acta Cryst B (1999), 000, 000-000. 3.- E. Espinosa, E. Molins and C. Lecomte. Chem. Phys. Lett. (1998), **285**, 170-173. 4.- E. Espinosa, C. Lecomte and E. Molins. Chem. Phys. Lett. (1999), 300, **745**-748.

Scientific Programme

The conference is divided in 3 sessions and consists of invited talks, short communications and poster presentations.

Sessions, invited speakers and talks (tentative titles) are:

Session A: *Intermolecular interactions*
(30/9/99)

Gastone Gilli (University of Ferrara):
"Towards a comprehensive model of hydrogen bond interaction".

Emilio Artacho (Universidad Autnoma de Madrid):
"Electron density in dry DNA from first-principles".

Bo Iversen (University of Aarhus):
"The electronic nature of strong hydrogen bonds: Implications for enzymatic catalysis".

Carlo Gatti (University of Milano):
"Weak cooperative electron-electron or molecule-molecule interactions in inorganic and organic crystals. A Quantum Theory of Atoms in Crystals approach".

Session B: *Other methods: spin and momentum densities*
(1/10/99)

Pierre Becker (Ecole Centrale Paris):
"Modelling charge and momentum densities, beyond the independent particle model.

Batrice Gillon (LLB-CEA, Saclay):
"Spin densities studies in molecular compounds: Polarized neutron diffraction".

Session C: *X-ray diffraction on materials under external perturbations*
(2/10/99)

Ullrich Pietsch (University of Potsdam):
"Electric field induced charge density variations in covalently bonded binary compounds".

Heinz Graafsma (E.S.R.F., Grenoble):

"Electric field induced structural changes in KDP and DKDP".

Poster presentation

The posters will be placed close to the ECDM-II lecture room. Posters can be set up on the panels since registration on Wednesday 29th. At least one of the authors is expected to be present during the whole poster session (Thursday 30th , from 18:30h to 20:00h) for presentation and discussion of the work. The Organising Committee encourages authors to keep their posters exposed during the whole meeting in order to promote discussions at any moment. For that purpose, coffee breaks will take place in the posters room. Posters must fit into a rectangle 90cm wide by 170cm high; posting supplies will be provided.

Poster communications are opened to any topic related to electron densities.

Social Events

- Welcome party: A cold buffet will be offered on Wednesday evening.

- Excursion: On Friday, October the 1st, a visit to Bodegas Torres in Vilafranca del Peneds (20 Km away from Sitges) is scheduled after the lunch. There, you will have a tour around the winery and the "Bodegas Torres" museum; a tasting of some of their products is included.

- Conference Dinner: It will take place at the Calpolis Hotel on Friday the 1st at 21:00h.

Important Dates

Pre-registration deadline:	15th December 1998
Abstracts deadline:	15th May 1999
Deadline for early registration payment (reduced rate):	31st May 1999
Deadline for registration payment:	31st July 1999
Deadline for 100cancelled registration fee (after,no refund will be possible):	31st August 1999

Registration fee

Registration fee covers: the conference fee, abstract book, excursion, conference dinner and accommodation (full board, room and all meals from Wednesday dinner to Saturday lunch) at the Calpolis Hotel (****). Fees for accompanying persons include the same except the conference fee and the abstract book. All ECDM-II attendees, including invited speakers, must register.

To be eligible for the reduced registration fee, payments should be received before 31st May

1999.

A limited number of grants for students is intended (the applications should be sent preferably by e- mail to the Organising Committee at the address **ecdmii@icmab.es** before 15/5/99).

Registration fee:

	Before 31/5/99	After 31/5/99
Double-room/single occupancy		
Attendee	70.000 Ptas. (420,71 Euros)	80.000 Ptas. (480,82 Euros)
Accompanying person	65.000 Ptas. (390,66 Euros)	75.000 Ptas. (450,76 Euros)
Double-room/double occupancy/person		
Attendee	55.000 Ptas. (330,56 Euros)	65.000 Ptas. (390,66 Euros)
Accompanying person	50.000 Ptas. (300,51 Euros)	60.000 Ptas. (360,61 Euros)

Registration fee should be paid in Ptas. by bank transfer to:

If you are abroad:

Swift: CAIX ES BB BCI
Branch: 0424
Account: 0200175633
Account name: ECDM-II
Bank name: Caixa d'Estalvis i Pensions de Barcelona
Address: Campus Universitat Autnoma de Barcelona
Edifici Rectorat
08193 Cerdanyola (Barcelona)
SPAIN

If you are in Spain:

Account: 2100-0424-35-0200175633
Account name: ECDM-II
Bank name: Caixa dEstalvis i Pensions de Barcelona
Address: Campus Universitat Autnoma de Barcelona
Edifici Rectorat
08193 Cerdanyola (Barcelona)
SPAIN

Please, **write your full name** in the bank transfer subject.

All payments must be made free of transfer charges/bank costs.

Final registration form should be filled in as early as possible by means of the ”On-line Registration” available in this website.

A copy of the bank transfer form should be sent to: ECDM-II / Secretariat (see the full address in our homepage) by regular mail.

Cancellations policy for registration and accommodation:

The cancellation received in writing prior August 31st 1999 will have full refund fee. No refunds will be issued after September 1st 1999. Reimbursements will be forwarded between 30 to 60 days after cancellation is received.

Useful information

Travel Information:

- Train: From El Prat International Airport there is a regular train service to Sitges: the Airport Railway Station is opposite Terminal A, (access to walkway between Terminals ”A” and ”B”). The single fare from the Airport- El Prat de Llobregat- Sitges is 235 Ptas. It is necessary to change trains at El Prat de Llobregat as follows:

a) Airport Station to El Prat de Llobregat Station (average journey 6 minutes). Trains depart from the Airport every half hour at 13 and 43 minutes past the hour. The first service is at 6h13m, the last at 22h13m. b) El Prat de Llobregat to Sitges (average journey 26 minutes). Trains depart from El Prat de Llobregat every 20 and 50 minutes past the hour. The first service is at 5h50m , the last at 23h20m.

- Taxi: An average journey by taxi from the Airport to Sitges should take 20 minutes, and depending on traffic, the cost of the ride should be around 6.000 Ptas. (36 Euros) with the motorway toll and baggage included.

Passport/Visa:

All foreign visitors to Spain must possess an identity card or passport. Participants requiring a visa should apply to consular offices or diplomatic missions in their country. For details, participants are advised to consult their local travel agencies.

For details on how to get to Calpolis Hotel from the Sitges rail station please see the map on the web site. There also details on the meeting schedule can be found.

Dr. Enrique Espinosa
Organising Committee ECDM-II / Secretariat
Instituto de Ciencia de Materiales de Barcelona (CSIC)
Campus de la UAB
08193 Cerdanyola (Barcelona), Spain
Tf: +34 93 5801853, Fax: +34 93 5805729, E-mail: enrique@icmab.es

MEETING ANNOUNCEMENT

6.3 The Materials Modelling Laboratory Workshop (MML'99)

1-4th September 1999
Department of Materials, University of Oxford

This 4 day workshop will cover materials modelling across the length scales including:

Talks on:
Density Functional Theory
Molecular Dynamics
Monte Carlo Methods
Phase Field
Dislocation Dynamics
Finite Element Methods
Finite Difference Methods
Multiscale Modelling
- Bridging the Length Scales

and
Tutorials on:
MSI software for electronic and atomistic methods
Equilibrium Thermodynamics (MTDATA)
Solidification Modelling

For further information and registration see:

http://users.ox.ac.uk/∼mml99/workshop.html

or e-mail: mml99@materials.ox.ac.uk.

The workshop is intended for non-specialists in these fields and will cover materials modelling across all the length scales. Participants from both industry and academia are most welcome. Student bursaries will be available for a number of students attending the workshop which will cover both registration and accommodation including meals. All students who attend the conference will be eligible for a reduced registration fee for the CCP5 meeting in Birmingham September 5-8. See: http://www.dl.ac.uk/CCP/CCP5/meetings/ann991.html for details. We

would like to acknowledge partial funding from CCP5.

Important Dates:

1st June	Registration deadline
8th June	Notification of acceptance and financial aid decisions
17th July	Payment deadline

Dr Steven Kenny (MML'99)
Department of Materials,
University of Oxford,
Parks Road,
Oxford,
OX1 3PH,
UK.

e-mail mml99@materials.ox.ac.uk

MML'99 Workshop Programme

Wednesday 1 September: Electronic Structure			
14:00	Steven Kenny	Plane waves	CoSi2 surface reconstructions
14:50	Duc Nguyen-Manh	LMTO/TB	T.B.A.
15:40	Coffee Break		
16:00	Sergei Dudarev	LSDA + U	Strongly correlated oxides
16:50	Dave Bowler	Density Matrix Methods	T.B.A.
Thursday 2 September: Atomistic Modelling			
9:30	Robert Rudd	Molecular Dynamics	T.B.A.
10:20	Mike Fearn	Monte Carlo	CVD of silicon/diamond
11:10	Coffee Break		
11:30	Ivan Oleinik	Reaction Pathways and Rates	Reactions on the diamond surface during CVD
12:30	Lunch		
14:30	MSI, Inc.	Software Demonstration and Tutorial	

Friday 3 September: Microstructural Modelling			
9:30	Adrian Sutton	Phase Field	T.B.A.
10:20	Ladislas Kubin	Kubin Model	T.B.A.
11:10	Coffee Break		
11:30	Steve Roberts	Dislocation dynamics	T.B.A.
12:30	Lunch		
14:30	Rachel Thomson	MTDATA equilibrium thermodynamics packages tutorial	
16:30	John Hunt	Solidification software tutorial	
19:30	Banquet		
Saturday Morning 4 September: Continuum Modelling			
9:30	Fionn Dunne	Finite Elements	Mechanical properties
10:20	Patrick Grant	Finite Difference	Process modelling of metals
11:10	Coffee Break		
11:30	Paul Buckley	Constitutive equations	Process modelling of polymers
12:30	Lunch		
Saturday Afternoon 4 September: Linking the Length Scales			
14:30	David Pettifor	electronic to atomistic	Removing the electronic degrees of freedom: Bond Order Potentials
15:20	Gerhard Goldbeck-Wood	atomistic to mesoscale	Removing the atomic degrees of freedom: grouping atoms in units
16:10	Coffee Break		
16:30	Robert Rudd	atomistic to continuum	Removing the atomic degrees of freedom in finite elements at the periphery

T.B.A. = To be announced

7 General Job Announcements

At the Institut für Geowissenschaften der Universität Kiel a **3-year Post-Doc Position**

is available in the framework of a research group concerned with the investigation of sulfide and selenide misfit layer compounds. The research group is funded by the German Science Foundation (DFG).

The position is for the investigation of structure-property-relations by atomistic models. The post-doc will be part of the 'Computational Crystallography' group. We are looking for a researcher with experience in quantum mechanical and perhaps empirical modelling of complex structures. Preference will be given to candidates with experience in DFT calculations. The candidate will be expected to strongly collaborate with several experimental groups in chemistry, physics, crystallography and material sciences and a theoretical group in physics.

The salary is according to BAT IIa (full-time). A prolongation is possible, subject to the continuation of funding through the German Science Foundation.

Applications should reach us before **1st July** and are to be sent to

Prof. W. Depmeier
Institut für Geowissenschaften
Mineralogie/Kristallographie
Universität Kiel
D-24098 KIEL
GERMANY
wd@min.uni-kiel.de

Additional information may be requested from B. Winkler, bjoern@min.uni-kiel.de

DOCTORAL POSITIONS

in theoretical Solid State Physics

Laboratoire de Théorie du Solide
Institut de Physique Appliquée, EPF–Lausanne, Switzerland

The Laboratoire de Théorie du Solide of EPFL invites applications for two graduate research assistantships in the area of the physics of metal surfaces and metal/semiconductor interfaces. The successful candidates will study atomic scale phenomena at surfaces or interfaces using first principles computational methods and develop models for the quantitative description of the corresponding macroscopic behavior. Applicants should hold an undergraduate degree in physics. They should also possess programming experience and a solid background in solid-state physics.

The two appointments are expected to start in the Summer of 1999. Interested candidates should submit their curriculum vitae, together with the name and address of two references, as soon as possible.

Prof. A. Baldereschi, Tel: +41-21-693 4445

Dr. N. Binggeli, E-mail: binggeli@dpmail.epfl.ch, Tel: +41-21-693 4477

Laboratoire de théorie du solide
Institut de Physique Appliquée
Ecole Polytechnique Fédérale
PHB–Ecublens, 1015 Lausanne, Switzerland
Fax: +41-21-693 4444

THE UNIVERSITY OF BIRMINGHAM

APPOINTMENTS in PHYSICAL CHEMISTRY

Applications are invited for two new positions in the School of Chemistry, which received a Grade 5 in the last Research Assessment Exercise. Candidates with research interests in any area of physical chemistry, chemical physics, or theoretical chemistry will be welcomed, although preference may be given to applicants whose interests will broaden the present research base in the Physical Chemistry section of the School. Applications are invited from candidates at different stages of their careers; that is, from those with established positions seeking to advance their careers, as well as those seeking their first tenured position.

The successful applicants will be expected to initiate and develop strong research programmes and to teach at both undergraduate and postgraduate levels. It is hoped to have both appointees in post by the start of next academic year. The closing date for applications is June 11, 1999.

Further particulars may be obtained from:

Staffing Services
The University of Birmingham
Edgbaston, Birmingham B15 2TT
Tel: 0121-414-6486; fax: 0121-414-4802;
E-mail: h.h.luong@bham.ac.uk

Informal enquiries can be made to:

Professor Ian W.M. Smith FRS at the School of Chemistry
Tel: 0121-414-4422; fax: 0121-414-4426;
E-mail: i.w.m.smith@bham.ac.uk

or

Professor Peter P. Edwards FRS Head of the School of Chemistry
Tel: 0121-414-4379; fax: 0121-414-4403;
E-mail: p.p.edwards@bham.ac.uk

The above information, along with further particulars, is available on the web at:

http://chemwww.bham.ac.uk/positions/physchem.htm

Georgetown University, Washington DC
Postdoctoral Fellow Position

The condensed matter theory group at Georgetown University has an opening for a postdoctoral fellow in the area of electronic structure theory. The group, consisting of myself, Jim Freericks, and Joe Serene, has overlapping interests in superconductivity, electronic correlations, and magnetism. The successful candidate will work most closely with me on projects related to linear and non-linear response in solids, electron-phonon interactions, and thermal and transport properties. The position will be available starting in the Fall of 1999. The initial appointment will be for two years, with a possible extension for a third year.

Your help in distributing this announcement to interested parties is greatly appreciated.

Amy Y. Liu	liu@physics.georgetown.edu
Assistant Professor of Physics	
Georgetown University	202-687-6583 (voice)
Washington, DC 20057	202-687-2087 (fax)

8 Abstracts

Charge transfer variation by symmetry breaking in a mixed-stack organic compound :TTF-2,5Cl_2BQ

C. Katan and C. Koenig
Groupe Matière Condensée et Matériaux (UMR-CNRS 6626),
Université Rennes-1, 35042 Rennes-Cedex, France

Abstract

In the "neutral to ionic" transition presented by some mixed-stack organic compounds, the inter-molecular charge-transfer variation at the critical pressure or temperature results both from the loss of inversion-symmetry and the lattice-contraction. We present here a 3-dimensional ab-initio study of the electronic ground-state of one of these charge-transfer salts: Tetrathiafulvalene-2,5-dichloro-p-benzoquinone, and discuss the relative importance of the intra- and inter-chain quantum interactions. Within a tight-binding scheme fitted to the self-consistent results, we show that the weak molecular distortions due to the symmetry-breaking part of the "neutral to ionic" transformation induce a non-negligible contribution to the total charge transfer variation.

(Accepted, J. of Phys.: Condensed Matter)
Manuscripts available from: Claudine.Katan@univ-rennes1.fr

First-principles study of the structures and vibrational frequencies for tetrathiafulvalene TTF and TTF-d_4 in different oxidation states

C. Katan
Groupe Matière Condensée et Matériaux (UMR-CNRS 6626),
Université Rennes-1, 35042 Rennes-Cedex, France

Abstract

The structures and vibrational spectra of tetrathiafulvalene (TTF), TTF-d_4 and their radical cations have been extensively studied using the Projector Augmented Wave method, which allows first-principles molecular dynamics based on the density functional theory. The dependence of the bond lenghts and vibrational frequencies on the molecular ionicity is discussed, and the ionization energy, Coulomb repulsion and spin-splitting parameter are also derived.

(Accepted, J. Phys. Chem. A)
Manuscripts available from: Claudine.Katan@univ-rennes1.fr

Canted spin structures in Ni films on stepped Cu(001)

S. S. Dhesi, H. A. Dürr and G. van der Laan
Daresbury Laboratory, Warrington WA4 4AD, United Kingdom

Abstract

We monitored the spin reorientation transition in ultrathin Ni films grown on a stepped Cu(001) surface with 3-dimensional magnetometry using magnetic circular x-ray dichroism signal at the Ni $L_{2,3}$ edge. We demonstrate that Ni films between 5.5 and 7 ML exhibit canted-spin structures, which include an angle of 20 - 30° with the surface normal. The transition from in-plane to perpendicular magnetic anisotropy is accompanied by a 90° in-plane spin rotation resulting in an orientation perpendicular to the step edges.

(Phys. Rev. B, accepted)
Manuscripts available from: g.vanderlaan@dl.ac.uk

Magnetic linear dichroism in Gd $4f$ and $4d$ photoemission of magnetic systems

Giancarlo Panaccione
APE Project INFM, Sincrotrone Trieste, I-34012 Basovizza, Trieste, Italy
Piero Torelli and Giorgio Rossi
INFM Dipartimento di Fisica dell'Università di Modena e Reggio Emilia, Modena, Italy
Gerrit van der Laan
Daresbury Laboratory, Warrington, WA4 4AD, United Kingdom
P. Prieto* and F. Sirotti
Laboratoire pour l'Utilisation du Rayonnement Electromagnétique, Orsay, France

Abstract

We present a combined experimental and theoretical study of magnetic linear dichroism in the angular distribution (MLDAD) of Gd $4f$ and $4d$ core level photoemission. Expressions are given for the spectral shape and photon energy dependence by using the method of fundamental spectra. The results are compared with experimental data for a thin Gd layer on Fe(100) and for a Fe/Gd/Fe interface. Compared to magnetic circular dichroism (MCD) in $4f$ photoemission, the MLDAD is much smaller and undergoes a sign change around 80 eV kinetic energy. We show that for $4f$ and $4d$ emission the spectral shapes of the MLDAD and MCD are in principle different, however in practise these differences are too small to observe.

(J. Phys. Condens. Matter, accepted)
Manuscripts available from: g.vanderlaan@dl.ac.uk

Pressure-induced isostructural phase transition in Al-rich NiAl alloys

Ali Alavi, Alexander Y. Lozovoi, and Michael W. Finnis
Atomistic Simulation Group, School of Mathematics and Physics,
Queen's University, Belfast BT7 1NN, U.K.

Abstract

We investigate the effect of elevated pressures and finite temperatures on the phase stability of Al-rich NiAl alloys. We use density functional theory to compute point-defect energies as a function of pressure, which are in turn used as input to an extended Wagner-Schottky model in which elastic interaction between defects is additionally allowed. We argue that this approach can be connected to regular solution theory. At elevated pressures, antisite Al defects are preferred to vacancies on the Ni sublattice. We show that the interactions between antisites and vacancies gives rise to lines of isostructural first-order phase transitions terminating at critical points. Implications of this type of behaviour for other ordered intermetallic compounds are discussed.

(Submitted to Phys. Rev. Lett.)
Manuscripts available from: m.finnis@qub.ac.uk

Do we really understand dislocations in semiconductors?

R. Jones
School of Physics, The University of Exeter, Exeter, EX4 4QL, UK

Abstract

The properties of dislocations in Si, GaAs and GaN are reviewed. Although, theoretical investigations favour a reconstruction eliminating, or reducing, the electrical activity in each case, with a consequent increase in the barrier for dislocation motion, there are problems in reconciling these results with experiment. It may be that the influence of impurities or point defects cannot be overlooked.

To appear Materials Science in Semiconductor Processing
Postscript and PDF files available from: jones@excc.ex.ac.uk.

Identification of the Hexavacancy in Silicon with the B^4_{80} Optical Center

B. Hourahine, R. Jones
School of Physics, The University of Exeter, Exeter, EX4 4QL, UK
A. N. Safonov
Department of Physics, University of Durham, South Road, Durham DH1 3LE, UK
S. Öberg
Department of Mathematics, University of Luleå, Luleå, S-97187, Sweden
P. R. Briddon
Department of Physics, The University of Newcastle upon Tyne,
Newcastle upon Tyne, NE1 7RU, UK
S. K. Estreicher
Department of Physics, Texas Tech University, Lubbock, Texas 79409-1051

Abstract

The ring hexavacancy (V_6) has been found by previous theoretical modeling to be a particularly stable defect, it has not been identified with any observed center. Here we use *ab initio* calculations to derive the structure and properties of two forms of V_6H_2 and identify these defects with the trigonal optical centers B_{41} and B^1_{71}, which are known to contain two hydrogen atoms in equivalent and inequivalent sites respectively. It follows from the calculations that V_6 should also be optically active and we identify it with the B^4_{80} (J-line) center.

Submitted to Physical Review Letters.
Postscript and PDF files available from: bh@excc.ex.ac.uk.

Raman scattering observations and *Ab initio* models of di-carbon complexes in AlAs

B. R. Davidson, R. C. Newman
Interdisciplinary Research Centre for Semiconductor Materials,
The Blackett Laboratory, Imperial College of Science, Technology and Medicine,
London, SW7 2BZ, UK
C. D. Latham, R. Jones
School of Physics, The University of Exeter, Exeter, EX4 4QL, UK
J. Wagner
Fraunhofer-Institut für Angewandte Festkörperphysik,
Tullastrasse 72, D-71908 Freiburg, Federal Republic of Germany
C. C. Button
Department of Electronic and Electrical Engineering, University of Sheffield,
Mappin Street, Sheffield, S1 3JD, UK
P. R. Briddon
Department of Physics, The University of Newcastle upon Tyne,
Newcastle upon Tyne, NE1 7RU, UK

Abstract

Raman scattering from an as-grown or annealed AlAs carbon δ-doping superlattice reveals lines at 1752 and 1856 cm^{-1}: the latter line shows the weaker intensity but has a resonant enhancement for incident light with an energy of 3 eV. These lines are comparable with those assigned to vibrational modes of two directly-bonded di-carbon centers in GaAs [J. Wagner *et al.* Phys. Rev. Lett. **78**, 74 (1997)]. First principles calculations are carried out to determine the structure and vibrational modes of di-carbon C–C defects located at various substitutional and interstitial sites in both AlAs and GaAs. The frequency of the C–C stretch mode is sensitive to the charge state and orientation and errors are not expected to exceed 10%. The di-carbon complex centered at an arsenic site is a deep donor and in its positively charged state is found to have axes aligned close to either $\langle 110 \rangle$ or $\langle 111 \rangle$ directions. The calculated frequencies and energies for the two orientations are essentially the same, so that these two structures offer an explanation for the observation of the two di-carbon Raman modes. An alternative assignment of one of the two observed modes to a different defect, such as an interstitial complex or neutral substitutional dimers, are considered but are ruled out as being incompatible with the experimental observations.

Submitted 22 April 1999 to Physical Review B
Latex, Postscript and PDF files available from: latham@excc.ex.ac.uk.

The diffusion of carbon in GaAs

C. D. Latham
School of Physics, The University of Exeter, Exeter, EX4 4QL, UK
M. Haugk
Technische Universität, Institut für Physik,
Theoretische Physik III, D-09107 Chemnitz, Germany
R. Jones
School of Physics, The University of Exeter, Exeter, EX4 4QL, UK
Th. Frauenheim
Universität-GH Paderborn, Theoretische Physik,
Fachbereich Physik, D-33098 Paderborn, Germany
P. R. Briddon
Department of Physics, The University of Newcastle upon Tyne,
Newcastle upon Tyne, NE1 7RU, UK

Abstract

Selfconsistent-charge density-functional tight-binding (*SCC-DFTB*) calculations have been performed to survey the potential energy surface for a single interstitial carbon atom introduced into GaAs. The results provided a possible model for the diffusion of carbon through GaAs with an activation energy of less than 1 eV. The carbon atom moves via split-interstitial and bond-centred configurations. Subsequently, the energetics of the model reaction were refined using a fully self-consistent density functional method, *AIMPRO.* These calculations were found to be in good agreement with the more approximate *SCC-DFTB* results. Experimental studies have also found an activation energy of ~ 1 eV for carbon migration in heavily doped material.

Submitted 12 May 1999 to Physical Review B
Latex, Postscript and PDF files available from: latham@excc.ex.ac.uk.

Self-Interstitial Clusters in Silicon

B. J. Coomer, J. P. Goss, A. Resende, and R. Jones
School of Physics, The University of Exeter, Exeter, EX4 4QL, UK
S. Öberg
Department of Mathematics, University of Luleå, Luleå, S-97187, Sweden
P. R. Briddon
Department of Physics, The University of Newcastle upon Tyne,
Newcastle upon Tyne, NE1 7RU, UK

Abstract

Local density functional calculations on the isolated silicon interstitial, I and its aggregates, I_2, I_3 and I_4 have been performed. Several geometries are considered for each aggregate and we report preliminary results on their energetically favourable structures. Two degenerate configurations are found for the di-interstitial possessing C_2 and C_i symmetry. The lowest energy tri-interstitial defect possesses C_{3v} symmetry and we propose that this defect is responsible for the W-optical centre observed in irradiated silicon. We confirm that the I_4 model proposed by Takeda *et al* [1] is a low energy, fully coordinated structure. 1. N. Aria and S. Takeda, Phys. Rev. Lett., **78**, 4265 (1997).

To appear in Materials Science in Semiconductor Processing
Postscript and PDF files available from: coomer@excc.ex.ac.uk.

Self-interstitial–hydrogen complexes in silicon

B. Hourahine, R. Jones
School of Physics, The University of Exeter, Exeter, EX4 4QL, UK
S. Öberg
Department of Mathematics, University of Luleå, Luleå, S-97187, Sweden
P. R. Briddon
Department of Physics, The University of Newcastle upon Tyne,
Newcastle upon Tyne, NE1 7RU, UK

Abstract

The vibrational properties of interstitial silane (SiH_4) and silyl (SiH_3) molecules in crystalline silicon are calculated using a first-principle, cluster based, spin-polarised local-density method. The Si-H stretch modes are found to be red-shifted by $\sim$ 300 cm^{-1} from those of the isolated molecule which lie around 2200 cm^{-1}. These results refute recent suggestions that modes observed around 2200 cm^{-1}, and previously assigned to hydrogenated vacancy defects, are due to these interstitial molecules.

To appear in Physical Review B – 15th June
Postscript and PDF files available from: bh@excc.ex.ac.uk.

Exchange and Correlation Kernels at the Resonance Frequency: Implications for Excitation Energies in Density-Functional Theory.

X. Gonze (1,2) and M. Scheffler (1)
(1) Fritz-Haber-Institut der Max-Planck-Gesellschaft,
Faradayweg 4-6, D-14195 Berlin-Dahlem, Germany
(2) Unite P.C.P.M., Universite Catholique de Louvain,
B-1348 Louvain-la-Neuve, Belgium

Abstract

Specific matrix elements of exchange and correlation kernels in time-dependent density-functional theory are computed. The knowledge of these matrix elements not only constraints approximate time-dependent functionals, but also allows to link different practical approaches to excited states, either based on density-functional theory, or on many-body perturbation theory, despite the approximations that have been performed to derive them.

(Accepted for publication in Phys. Rev. Lett. (scheduled 31 May 1999).)

Contact person: gonze@fhi-berlin.mpg.de

Arsenic Dimer Dynamics during MBE Growth: Theoretical Evidence for a Novel Chemisorption State of As_2 Molecules on GaAs Surfaces

C. G. Morgan[1,2], P. Kratzer[1], and M. Scheffler[1]
[1]*Fritz-Haber-Institut der Max-Planck-Gesellschaft,*
Faradayweg 4-6, D-14195 Berlin-Dahlem, Germany
[2]*Physics Department, Wayne State University,*
Detroit MI 48202, U.S.A.

Abstract

Results of first-principles calculations are reported for the adsorption of As_2 molecules on the stable surface reconstructions of the GaAs (001) surface, including adsorption paths and barriers for strongly bound sites. It is shown that a novel chemisorption state acts together with an intermediate physisorbed plateau in the total energy to hold the As_2 molecules near the surface and funnel them into strongly bonding sites during epitaxial growth, and that this state can explain the transition from the $\beta 2(2\times4)$ to the c(4×4) reconstruction under low-temperature, very arsenic-rich conditions.

(Submitted to Phys. Rev. Lett. (December 1998).)

Contact person: morgan_c@fhi-berlin.mpg.de

Atomic exchange processes and *bimodal* initial growth of Co/Cu(001)

F. Nouvertné, U. May, M. Bamming, A. Rampe, U. Korte, G. Güntherodt
2. Physikalisches Institut der RWTH Aachen, D-52056 Aachen, Germany
R. Pentcheva and M. Scheffler
Fritz-Haber-Institut der Max-Planck-Gesellschaft,
Faradayweg 4-6, D-14195 Berlin-Dahlem, Germany

Abstract

The initial growth of Co on Cu(001) is studied by scanning tunneling microscopy (STM) experiments and density-functional theory total-energy calculations. The results reveal that at low coverage Co adatoms occupy substitutional sites in the Cu substrate surface which act as pinning centers for subsequent island nucleation. Theis atomic substitution process actuates a new *bimodal* growth mode giving rise to a high density of small Co islands and large Co-decorated Cu islands.

(Submitted to Phys. Rev. Letter (February 1998).)
Contact person: pentcheva@fhi-berlin.mpg.de

Towards a first-principles theory of surface thermodynamics and kinetics

C. Stampfl,[1] H. J. Kreuzer,[2] S. H. Payne,[2]
H. Pfnür,[3] and M. Scheffler,[1]
[1] *Fritz-Haber-Institut der Max-Planck-Gesellschaft,*
Faradayweg 4-6, D-14195 Berlin-Dahlem, Germany
[2] *Department of Physics, Dalhousie University, Halifax,*
Nova Scotia, B3H 3J5, Canada
[3] *Institut für Festkörperphysik, Universität Hannover,*
Appelstrasse 2, D-30176 Hannover, Germany

Abstract

Understanding of the complex behavior of particles at surfaces requires detailed knowledge of both macroscopic and microscopic processes that take place; also certain processes depend critically on temperature and gas pressure. To link these processes we combine state-of-the-art microscopic, and macroscopic phenomenological, theories. We apply our theory to the O/Ru (0001) system and calculate thermal desorption spectra, heat of adsorption, and the surface phase diagram. The agreement with experiment provides validity for our approach which thus identifies the way for a predictive simulation of surface thermodynamics and kinetics.

(Submitted to Phys. Rev. Lett. (May 3 1999).)
Contact person: stampflc@fhi-berlin.mpg.de

Formation and stability of self-assembled coherent islands in highly mismatched heteroepitaxy

L. G. Wang, P. Kratzer, M. Scheffler, and N. Moll
Fritz-Haber-Institut der Max-Planck-Gesellschaft,
Faradayweg 4-6, D-14195 Berlin-Dahlem, Germany

Abstract

We study the energetics of island formation in Stranski-Krastanow growth within a parameter-free approach. It is shown that an optimum island size exist for a given coverage and island density if changes in the wetting layer morphology after the 3D transition are properly taken into account. Our approach reproduces well the experimental island size dependence on coverage, and indicates that the critical layer thickness depends on growth conditions. The present study provides a new explanation for the (frequently found) rather narrow size distribution of self-assembled coherent islands.

Phys. Rev. Lett. **82**, 4042(1999).
Contact person: lgwang@fhi-berlin.mpg.de

Optimization of Gutzwiller Wavefunctions in Quantum Monte Carlo

Erik Koch and Olle Gunnarsson
Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart
Richard M. Martin
Department of Physics, University of Illinois, Urbana, IL 61801

Abstract

Gutzwiller functions are popular variational wavefunctions for correlated electrons in Hubbard models. Following the variational principle, we are interested in the Gutzwiller parameters that minimize e.g. the expectation value of the energy. Rewriting the expectation value as a rational function in the Gutzwiller parameters, we find a very efficient way for performing that minimization. The method can be used to optimize general Gutzwiller-type wavefunctions both, in variational and in fixed-node diffusion Monte Carlo.

(to be published in Phys. Rev. B; Latex-file available as `cond-mat/9903070`)

Screening, Coulomb pseudopotential, and superconductivity in alkali-doped Fullerenes

Erik Koch and Olle Gunnarsson
Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany
Richard M. Martin
Department of Physics, University of Illinois, Urbana, IL 61801, USA

Abstract

We study the static screening in a Hubbard-like model using quantum Monte Carlo. We find that the random phase approximation is surprisingly accurate almost up to the Mott transition. We argue that in alkali-doped Fullerenes the Coulomb pseudopotential μ^* is not very much reduced by retardation effects. Therefore efficient screening is important in reducing μ^* sufficiently to allow for an electron-phonon driven superconductivity. In this way the Fullerides differ from the conventional picture, where retardation effects play a major role in reducing the electron-electron repulsion.

(submitted to Phys. Rev. Lett.; Latex-file available as `cond-mat/9902241`)

Filling dependence of the Mott transition in the degenerate Hubbard model

Erik Koch and Olle Gunnarsson
Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany
Richard M. Martin
Department of Physics, University of Illinois, Urbana, IL 61801, USA

Abstract

Describing the doped Fullerenes using a generalized Hubbard model, we study the Mott transition for different integer fillings of the t_{1u} band. We use the opening of the energy-gap E_g as a criterion for the transition. E_g is calculated as a function of the on-site Coulomb interaction U using fixed-node diffusion Monte Carlo. We find that for systems with doping away from half-filling the Mott transitions occurs at smaller U than for the half-filled system. We give a simple model for the doping dependence of the Mott transition.

(submitted to Phys. Rev. B; Latex-file available as `cond-mat/9905351`)

Fully relativistic band structure calculations for magnetic solids
– Formalism and Application –

H. Ebert
Institut für Phys. Chemie, Univ. München,
Butenandtstr. 5-13, D-81377 München, Germany

Abstract

Relativistic effects, in particular the spin-orbit coupling, give rise for magnetic systems to a great number of interesting and technologically important phenomena. The formal and technical aspects of corresponding fully relativistic theoretical investigations are reviewed. The properties of the underlying Dirac equation, set up within the framework of density functional theory (DFT) are discussed together with the Breit-interaction and Brooks' orbital polarization mechanism. As an example for a corresponding band structure method, the Korringa-Kohn-Rostoker (KKR) Green's function method is adopted. In particular, some technical aspects specific to this technique are discussed. The numerous applications that will be presented are primarily meant to demonstrate the many different facets of relativistic – this means in general – of spin-orbit induced effects in magnetic solids. In addition, these also demonstrate the tremendous flexibility of band structure schemes based on the Green's function formalism.

This article will be published in: *The TB-LMTO-method*
edited by H. Dreysse, Springer series *Lecture Notes in Physics*, Springer Verlag, Berlin.
Manuscript available as ps-file on request from: H. Ebert (he@gaia.cup.uni-muenchen.de)

A Fully Relativistic Theory For Magnetic EXAFS – Formalism And Applications

H. Ebert and V. Popescu
Institut für Physikalische Chemie, Universität München,
Butenandtstr. 5-13, D-81377 München, Germany
D. Ahlers
Lehrstuhl für Experimentalphysik IV, Universität Würzburg,
Am Hubland, D-97074 Würzburg, Germany

Abstract

A fully relativistic theory for magnetic Extended X-ray Absorption Fine Structure (MEXAFS) is presented that is based on the Dirac equation for spin-polarized systems and relativistic multiple scattering theory. This scheme not only allows one to treat spin-polarization and all relativistic effects on the same level but can also be applied to go beyond the standard muffin-tin construction by using non-spherical potentials. To illustrate the application of the presented fully relativistic scheme, results for the K-edge spectra of Ni in fcc-Ni and the $L_{2,3}$-edges of Pt in fcc-Fe_3Pt are presented. A very simple and convincing interpretation of the corresponding dichroic spectra is given on the basis of the differential form of the so-called sum rules.

(Submitted to *Phys. Rev. B*)
Manuscript available as ps-file on request from H. Ebert (he@gaia.cup.uni-muenchen.de)

A fully relativistic description of the magneto-optical properties of arbitrary layered systems

T. Huhne, H. Ebert
Institut für Physikalische Chemie, Universität München,
Butenandtstr. 5-13, D-81377 München, Germany

Abstract

A fully relativistic formalism is presented that allows to define the freqency-dependent optical conductivity tensor for arbitrary layered systems in a layer-resolved way. This opens in particular the way to deal with the magneto-optical properties of magnetic surface layer systems and to calculate the corresponding magneto-optical Kerr spectra. The formalism, based on a fully relativistic description of response theory in arbitrary order, is described in some detail. For an implementation the very flexible spin polarized relativistic Korringa-Kohn-Rostoker (SPR-KKR) method of band structure calculation has been used. First results of corresponding applications to the elemental ferromagnets bcc-Fe and fcc-Co treated as homogeneous layer systems are presented.

(Submitted to *Phys. Rev. B*)
Manuscript available as ps-file on request from H. Ebert (he@gaia.cup.uni-muenchen.de)

9 SCIENTIFIC HIGHLIGHT OF THE MONTH

Quasi-particles and Van Hove Scenario for the Superconducting Cuprates

B L Gyorffy
H H Wills Physics Laboratory, University of Bristol,
Tyndall Avenue, Bristol, BS8 1TL, UK
Z Szotek and W M Temmerman
Daresbury Laboratory, Daresbury, Warrington, WA4 4AD, UK
O K Andersen and O Jepsen
Max-Planck-Institut für Festkörperforschung, Postfach 800665,
D-70506, Stuttgart, Federal Republic of Germany
G Litak
Department of Mechanics, Technical University of Lublin, Nadbystrzycka 36,
PL-20-618 Lublin, Poland
A Martin and J F Annett
H H Wills Physics Laboratory, University of Bristol,
Tyndall Avenue, Bristol, BS8 1TL, UK
K I Wysokinski
Institute of Physics, M. Curie-Sklodowska University, Radziszewskiego 10a,
PL-20-031 Lublin, Poland

The Van Hove Scenario

In the simplest, BCS, microscopic theory of superconductivity the gap Δ in the excitation spectrum of the superconducting state is the order parameter. At zero temperature it is determined by the gap equation [1]:

$$\frac{1}{u} = \int_{\varepsilon_F}^{h\omega_D+\varepsilon_F} d\varepsilon \frac{N(\varepsilon)}{2\sqrt{(\varepsilon-\mu)^2+\Delta^2}}, \tag{9.1}$$

where $N(\varepsilon)$ is the normal state density of states, $\mu \cong \varepsilon_F$ is the chemical potential, ε_F is the Fermi energy, ω_D is the Debye frequency, and u is the coupling constant which describes the strength of the electron-electron attraction. Here $h = h/2\pi$. Usually, $N(\varepsilon)$ does not vary much on the small energy scale of eV and thus it may be replaced in Eq. (9.1) by its value at the Fermi energy, $N(\varepsilon_F)$, independent of ε. Then Eq. (9.1) can be solved and one finds the well known result that $\Delta \approx 2\ h\ \omega_D \exp(-\frac{1}{uN(\varepsilon_F)})$. Evidently, this argument breaks down if $N(\varepsilon)$ varies rapidly on the scale of $h\omega_D$, as it would for ε_F near a Van Hove singularity (VHS). Typically, such a singularity is defined by $\bar{\bigtriangledown}\varepsilon_{\mathbf{k}} = 0$ and leads to a logarithmic dependence, $N(\varepsilon) \cong \ln(\varepsilon - \varepsilon_{VHS})$, of the density of state in Eq. (9.1). This changes the solution of Eq. (9.1) dramatically giving rise to a significantly larger gap Δ than the famous BCS result above. Since $k_B T_c \cong \Delta$, the larger gap Δ implies larger transition temperature T_c, and hence we conclude that T_c is enhanced if, without changing the coupling constant u, ε_F approaches the Van Hove singularity at ε_{VHS}.

As was noted by Friedel [2] and Markiewicz [3, 4] the above enhancement, which could be as much as a factor of 5 to 10, of T_c may have an important role to play in the explanation of high T_c superconductivity. In short, they have argued that whatever is the mechanism of attraction, it may be of modest strength if T_c is enhanced by the nearness of ε_F to ε_{VHS}. Over the last 10 years this Van Hove Scenario retained and even increased its attraction for two reasons. Firstly, the salient empirical fact about the high T_c superconductors turned out to be the rise and fall of T_c with the carrier concentration n, namely doping. Evidently, such behaviour can be readily explained if we assume that on doping ε_F approaches and then passes a Van Hove singularity at ε_{VHS} [4]. Secondly, in the first-principles, parameter free, calculations of the electronic structure, for most high temperature superconductors a Van Hove singularity was found near ε_F [5]. The point of this contribution is to highlight recent developments, which goes beyond merely noting that high T_c occurs in materials with ε_{VHS} near ε_F, and to report on results of actual calculations of T_c as a function of doping.

Semiphenomological Models of the Attractive Interactions

In a first-principles calculation of the electronic structure in the normal state one often seeks the wave function in the form

$$\psi_\nu(\mathbf{r}) = \sum_{L,R} \psi^\nu_{L,R} \phi_L(\mathbf{r} - \mathbf{R}), \tag{9.2}$$

where L and $\mathbf{R}$ label a complete set of orthogonal orbitals and the lattice sites, respectively, and solves an energy eigenvalue equation for the amplitudes $\psi^\nu_{L,R}$:

$$\sum_{L',R'} H_{LR,L'R'} \psi^\nu_{L',R'} = E_\nu \psi^\nu_{L,R}. \tag{9.3}$$

In the superconducting state an excitation has an amplitude, $u_\nu(\mathbf{r})$, that is a particle and another, $v_\nu(\mathbf{r})$, that is a hole and these two satisfy a coupled set of Bogoliubov-de Gennes equations [4].

The analogue of Eq. (9.2) is the expansion [6]

$$\left[\begin{array}{c} u_\nu(\mathbf{r}) \\ v_\nu(\mathbf{r}) \end{array}\right] = \sum_{RL} \varphi_L(\mathbf{r}-\mathbf{R}) \left[\begin{array}{c} u^\nu_{RL} \\ v^\nu_{RL} \end{array}\right]. \tag{9.4}$$

where the spinor $\left[\begin{array}{c} u^\nu_{RL} \\ v^\nu_{RL} \end{array}\right]$ satisfies the Bogoliubov-de Gennes equations:

$$\sum_{RL} \left[\begin{array}{cc} H_{R'L',RL} - \mu\delta_{R'L',RL} & \Delta_{R'L',RL} \\ \Delta^*_{RL,R'L'} & -H_{R'L',RL} + \mu\delta_{R'L',RL} \end{array}\right] \left[\begin{array}{c} u^\nu_{RL} \\ v^\nu_{RL} \end{array}\right] = E_\nu \left[\begin{array}{c} u^\nu_{RL} \\ v^\nu_{RL} \end{array}\right]. \tag{9.5}$$

which is the analogue of Eq. (9.3). The pairing potential, which in the simple BCS theory is the gap Δ, can be calculated from the pairing amplitude:

$$\chi_{RL,R'L'} \equiv \sum_\nu \left[1 - f(E_\nu)\right] u^\nu_{RL}\, {v^\nu_{R'L'}}^* - f(E_\nu)\, u^\nu_{R'L'}\, {v^\nu_{RL}}^*, \tag{9.6}$$

using the relation:

$$\Delta_{RL,R'L'} = \sum_{R_1L_1} \sum_{R_1'L_1'} K_{RL,R'L';R_1L_1,R_1'L_1'}\ \chi_{R_1L_1,R_1'L_1'}, \tag{9.7}$$

where the kernel K describes the electron-electron attraction.

In the normal state H depends on the amplitudes $\psi^\nu_{L,R}$. For instance this relationship may be that implied by the Local Density Approximation (LDA). Thus, as is well known, Eq. (9.3) is a self-consistant field problem. Typically, solving the Kohn-Sham equation using the LMTO method takes this form.

It turns out that Eq. (9.5), which describes the superconducting ground state, can also be regarded as a Kohn-Sham equation of density functional theory with the apropriate broken (gauge) symmetry. In fact this theory is analogous to spin-density functional theory with the pairing amplitude, χ, replacing the magnetization density m as the order parameter.

Evidently, the principle new feature of the superconductivity problem is the interaction kernel K, which is largely unknown. Nevertheless, progress can be made by parametrizing it in terms of phenomenological constants [6]. In fact what appears to be a useful approach is to simplify Eq. (9.7) by keeping only the diagonal parts of K and using the coefficients in

$$\Delta_{RL,R'L'} = K_{RL,R'L'}\ \chi_{RL,R'L'}, \tag{9.8}$$

as adjustible parameters. In any given practical calculations, so far, only one of these parameters was allowed to be nonzero and its value was fixed by demanding that the critical temparature T_c, above which $\chi_{RL,R'L'}$, and therefore $\Delta_{RL,R'L'}$, work out to be zero, agrees with experiments. In short, the strategy for calculating the electronic structure in the superconducting state is to take a Hamiltonian matrix (function of the amplitudes and orbitals) which works well in the normal state and add to it the one parameter (K) pairing potential Δ.

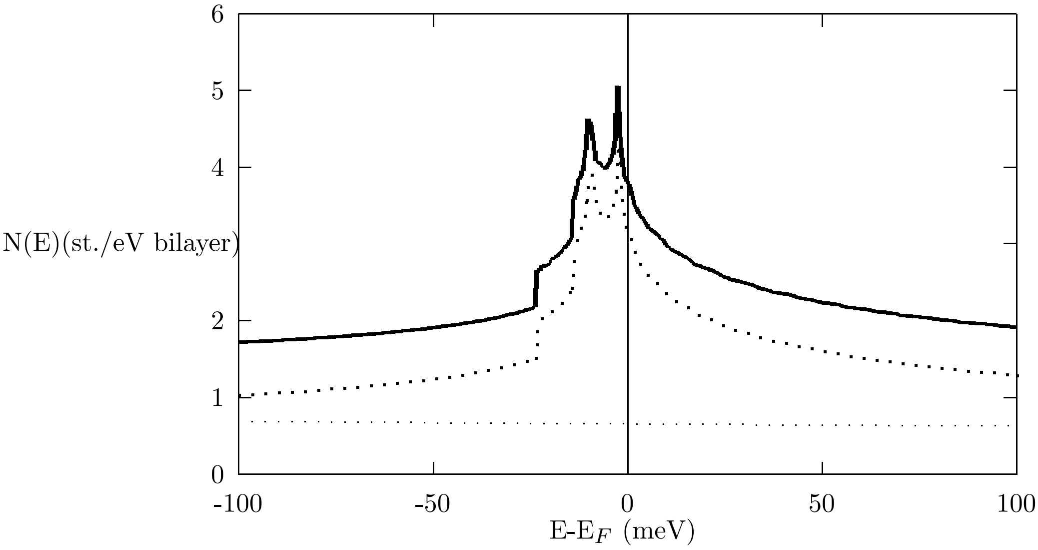

Figure 1: The normal-state density of states in the neighbourhood of the Fermi level for the eight odd (thick dots) and eight even (thin dots) CuO_2 plane-bands of $YBa_2Cu_3O_7$, as well as their sum (full curve). The two logarithmic van Hove singularities are due to the saddle-points of the odd plane-band near respectively X and Y. Here 'odd' and 'even' refer to the symmetry of the wave functions with respect to the mirror plane between the two CuO_2 layers of the bilayer.

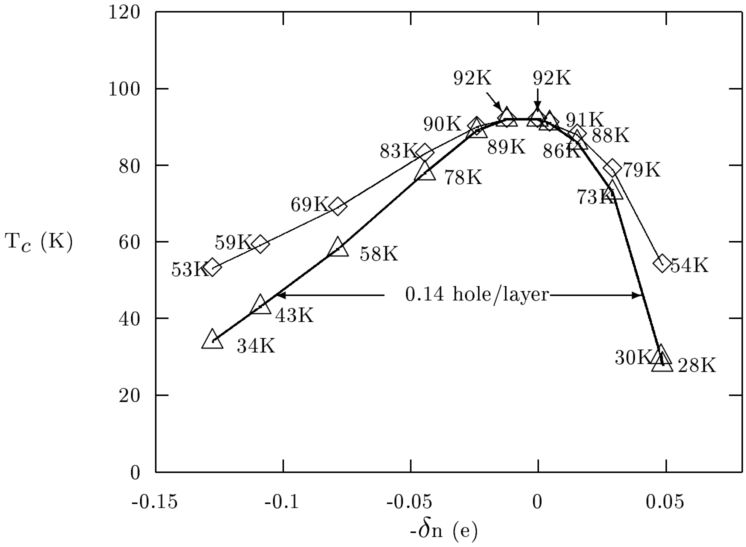

Figure 2: T_c versus deviation of the number of holes from that at optimal doping for the CuO_2 bilayer of $YBa_2Cu_3O_7$. The thick solid curve with triangles corresponds to the intra-layer nearest-neighbour Cu $d_{x^2-y^2}$−Cu $d_{x^2-y^2}$ scenario ($d-$wave superconductivity), while the thin solid curve with diamonds represents the on-site Cu $d_{x^2-y^2}$−Cu $d_{x^2-y^2}$ scenario ($s-$wave superconductivity). On both curves T_c's corresponding to different hole concentrations are marked.

T$_c$ versus Doping

The first implementation of the above procedure [6, 7] was based on H corresponding to the eight-band model of Andersen *et al.* [8] for the high T_c cuprates ($YBa_2Cu_3O_7$). Interestingly, from the point of view of our present concern the bands resulting from this H featured a prominent (bifurcated) Van Hove singularity. A consequence of this is the two sharp peaks in the density of states shown in Fig. 1.

On introducing the electron-electron attraction, the scenario which turned out to be most interesting was the one in which the interaction, K, operated between electrons, with opposite spins, on nearest neighbour Cu sites, occupying $d_{x^2-y^2}$ orbitals. The coupling constant which gives T_c=92K turned out to be K=0.68 eV. With this one phenomenological constant fixed, a number of other physical properties, such as the low temperature specific heat and the quasi-particle spectra, were calculated in good, quatitative agreement with experiments [6].

At this stage the scene was set to investigate the influence of Van Hove singularities on the superconducting properties in the context of a realistic description of the electronic structure in the normal state. To mimic the effects of doping the chemical potential was changed as one would in making a rigid band argument but of course the interaction constant K was kept the same. The very encouraging result for the T_c vs. doping is shown in Fig. 2. Evidently, the Van Hove scenario works and, suprisingly, the width of the peak is in good agreement with the width of 0.15 holes per layer found empirically.

Effects of Disorder

A serious, general, objection one can raise against the above arguments is that doping, inevitably, brings with it disorder which will smear out, and render ineffective, the Van Hove singularity. To investigate the force of this criticism Litak *et al.* [9] have studied the effect of disorder scattering on the Van Hove scenario on the basis of a model with reduced realism. In fact, they have used a one band, extended, negative U Hubbard model which, in the Hartree-Fock-Gorkov approximation, gave rise to a simplified version of the Bogoliubov-de Gennes equation in Eq. (9.5). The disorder was introduced into the problem by allowing the site energies, ε_i, to take values $\delta/2$ and -$\delta/2$ randomly, and it was treated in the Coherent Potential Approximation (CPA) [10]. The calculations were performed for nearest neighbour hopping on a square lattice for which the normal state featured the well known prototype of Van Hove singularity at the band center. The way the corresponding peak is smeared by disorder is illustrated in in Fig. 3, where we show the density of states for different strength, δ, of disorder as calculated by the CPA procedure in the normal state.

Thus the question is "how does this gradual broadening of the central peak affects the doping dependence of the transition temperature T_c?". For the particular case at hand this is answered in Fig. 4 where we show the results of the CPA calculation for the superconducting state.

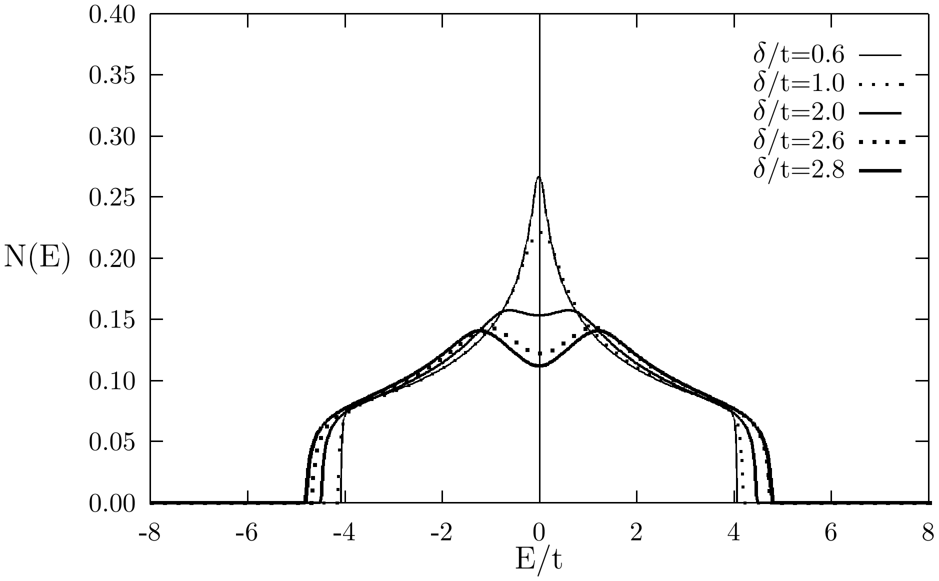

Figure 3: Density of states $N(E)$ for a normal state with various disorder strengths $\delta = \epsilon_A - \epsilon_B$ ($A_{0.5}$ $B_{0.5}$).

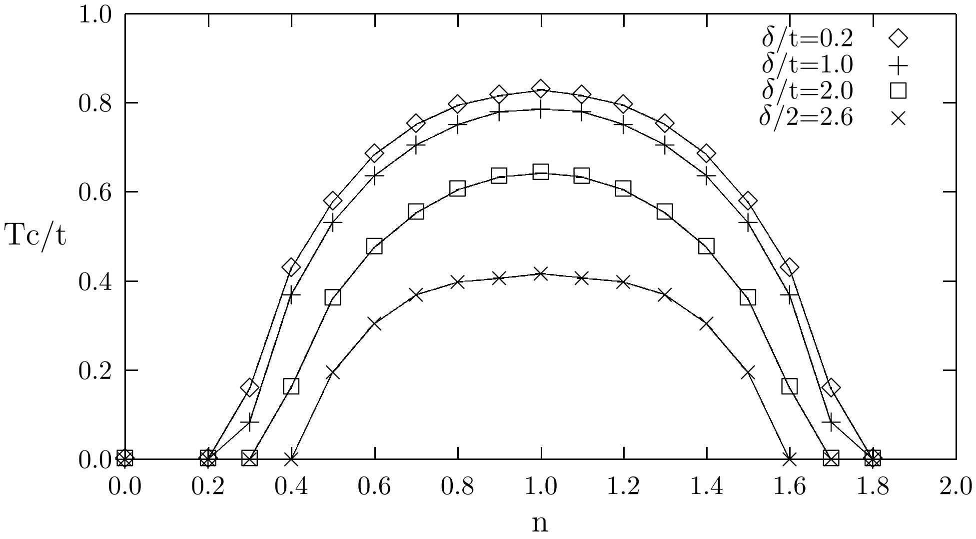

Figure 4: Critical temperature T_c vs. band filling n for d wave superconductors with a number of disorder strengths δ.

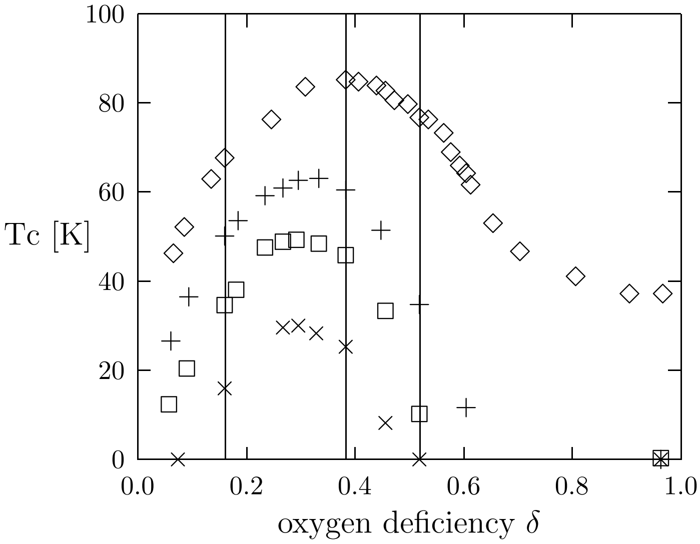

Figure 5: Critical temperature T_c as a function of oxygen deficiency δ for $Y_{0.8}Ca_{0.2}Ba_2(Cu_{1-y}Zn_y)_3O_{7-\delta}$ with $y = 0$ ($\diamond$), $y = 0.02$ ($+$), $y = 0.04$ ($\square$), $y = 0.06$ ($\times$) [11].

Evidently, with increasing disorder the enhancement of T_c by the Van Hove singularity fades gradually in agreement with the experiments depicted in Fig. 5. Thus, we conclude that simple calculations support the suggestion that the high T_c in the cuprates comes about as a result of a relatively weak pairing force being enhanced by the closeness of a Van Hove singularity to the Fermi energy.

References

[1] M.Tinkham, 'Introduction to Superconductivity' (Second eddition Krieger, 1980).

[2] J. Friedel, J. Phys. Condens. Matter **1** (1989) 7757.

[3] R.S. Markiewicz and B.C.Giessen, Physica C **160** (1989) 497.

[4] R.S. Markiewicz, J. Phys. Chem. Solids **58** (1997) 1173.

[5] D.L. Novikov and A.J.Freeman, in J. Klamut, B.W. Veal, B.M. Dabrowski, P.W. Klamut, M. Kazimierski (Eds.), 'Recent Developments in High Temperature Superconductivity' (Springer Verlag 1996).

[6] B.L. Gyorffy, Z. Szotek, W.M. Temmerman, O.K.Andersen, and O. Jepsen, Phys. Rev. B **58**, 1025-1042 (1998).

[7] Z. Szotek, B.L. Gyorffy, W.M. Temmerman, and O.K. Andersen, Phys. Rev. B **58**, 522-526 (1998).

[8] O.K. Andersen, O. Jepsen, A.I. Liechtenstein, and I.I. Mazin, Phys. Rev. B **49**, 4145 (1994).

[9] G. Litak, A.M. Martin, B.L. Gyorffy, J.F. Annett, K.I. Wysokinski, Physica C **309** (1998) 257-262.

[10] G. Litak, K.I. Wysokinski, R. Micnas, S. Robaszkiewicz, Physica C **199** (1992) 191.

[11] C. Bernhard, J.L. Tallon, C. Bucci, R. De Renzi, G, Guidi, G.V.M. Willians and Ch. Niedermayer, Phys. Rev Lett. **77**, 2304 (1996).