Ψ_k Newsletter

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

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Contents

1 Editorial

In this Psi-k Newsletter we have four reports on workshops, spread over three different sections: **RTN1**, **ESF**, and **CCP9**. All those workshops were partially supported by the ESF Programme, and all the reports contain abstracts of presented papers. In addition, in the **ESF Programme** section we have a report on a collaborative visit of Zs. Major (University of Bristol, UK) to Prof. H. Ebert (Munich University, Germany). General workshop/conference and open position announcements can be found in their usual sections, followed by the **Abstract** section with abstracts of newly submitted or recently published papers. The newsletter is finished with the scientific highlight by Mojmír Šob, Martin Friák, Dominik Legut (*Brno, Czech Republik*), and Václav Vitek (*Philadelphia, USA*) on **"Strength, magnetism and stability of metals and intermetallics at extreme loading conditions"**. Please check the table of contents for further details.

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

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

The above contains information on the Psi-k 2003 workshops and hands-on courses (subject to funding). In these pages you can also find information on how to apply for funding to make collaborative visits.

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**
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Dzidka Szotek and Walter Temmerman
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2 News from the Research Training Network 1 (RTN1)

COMPUTATIONAL MAGNETOELECTRONICS

2.1 Reports on RTN1 Workshops

2.1.1 Report on the International Workshop on "Diluted Magnetic Semiconductors"

CECAM, Lyon, June 12-14, 2003

Sponsors:

- ESF Ψ_k Programme "Towards Atomistic Materials Design"
- Centre Europén de Calcul Atomique et Moléculaire (CECAM)
- EU RT-Network "Computational Magnetoelectronics"
- Office of Naval Research, USA

Organisers:

- Peter H. Dederichs, Institut für Festkörperforschung, Research Center Jülich
- Josef Kudrnovský, Institute of Physics, Academy of Sciences, Prague
- Allan H. MacDonald, Department of Physics, University of Texas at Austin

Aim:

To strengthen the understanding of diluted magnetic semiconductors and bring together theorists from the ab-initio and model hamiltonian field with leading experimentalists.

The workshop took place close to the CECAM office in the Biology lecture hall of the ENS building. It was attended by 52 participants, among them eight from the USA, funded by ONR, and three from Japan. The workshop started with three longer introductory talks by Allan MacDonald on model Hamiltonians, Ilja Turek on density functional theory, and Peter Schiffer on experimental results. They were followed by 34 invited presentations, of either 30' or 20' length, and closed by a summary of Tomasz Dietl. While most of the participants were theorists, there were nevertheless 7 authoritive experimental reviews about the latest state of the art.

The workshop was very lively and well received. There were lots of discussions after practically every talk. The special discussion period forseen in the programme had even to be extended by two hours. For the first time a large number of theorists from all around the world joined in a workshop on this hot topic, discussing the physics of DMS and the success and problems of the model Hamiltonian approach on the one hand and the ab-initio approach on the other. The workshop was very informative and motivating and the general opinion was that we have still some way to go before we have a good understanding of the complicated systems and hopefully achieve ferromagnetism at room temperature.

Another point will make this workshop unforgetable for all participants: the weather. On all three days the temperature outside was 37-38 degrees Celsius, and not much less in the lecture hall, since air-conditioning was not available. Even the overhead projectors gave up because of overheating; at the end we had 5 projectors lined up in a row, three of them dead. However the participants stayed alive and active and even at the last talk of Tomasz Dietl on Saturday afternoon the room was well filled.

Peter H. Dederichs Phivos Mavropoulos

Programme

Thursday, June 12

		Overview Session
8:30	9:10	**A.H. MacDonald:** Theory of Magnetic Semiconductors
9:10	9:50	**I. Turek:** Exchange interactions and residual resistivity
9:50	10:30	**P. Schiffer:** Defect-Controlled Magnetism in (Ga,Mn)As
10:30	11:00	Coffee Break
		Mechanism
11:00	11:30	**M. van Schilfgaarde:** Role of Defects in DMS Alloys
11:30	12:00	**K Sato:** Exchange interactions and Curie temperatures
12:00	12:30	**T.C. Schulthess:** Mn impurities: from shallow to deep levels
12:30	14:00	Lunch
		Material Comparisons
14:00	14:20	**C. Timm:** Tight-binding theory for diluted ferromagnetic semiconductors
14:20	14:40	**J. Kurdnovsky:**Electronic and magnetic properties of GaMnAs alloys: ab-initio LDA+U study
14:40	15:00	**B. Sanyal:**Mn doped DMS - a comparative study
15:00	15:20	**Ph. Mavropoulos:** Half-metallic Zinc-blende Compounds and Multilayers with Semiconductors
15:20	15:40	**H. Akai:** Control on Hyperfine Interactions of Anti-Site As Through Bias Voltages
15:40	16:10	Coffee Break

Spin-Injection

16:10	16:40	**L.W. Molenkamp:** Spintronic Nanostructures
16:40	17:10	**B.T. Jonker:** Spin Injection from Ferromagnetic Semiconductors and Metals
17:10	17:40	**H. Jaffres:** Spin injection into semiconductors (theory and experiments)
17:40	18:10	**B. Beschoten:** Spin coherence and dephasing in n-GaAs across the metal-insulator transition

Friday, June 13

Defects and Magnetism

8:30	9:00	**S. Erwin:** Tale of Two Sites: Substitutional vs. interstitial doping in DMS
9:00	9:20	**V. Drchal:** Incorporation of Mn atoms into DMS
9:20	9:40	**F. Máca:** Compositional dependence of lattice constant and impurity formation energies in (Ga,Mn)As
9:40	10:05	**L. Sandratskii:** Electronic structure, exchange interactions and Curie temperature in DMS
10:05	10:30	**L. Bergqvist :** Magnetic and Electronic Structure of $(Ga_{1-x}Mn_x)As$
10:30	11:00	Coffee Break

Disorder and Frustration

11:00	11:20	**L. Brey:** Heisenberg-Like Hamiltonian for GaMnAs
11:20	11:40	**G. Zarand:** Magnetic Semiconductors: Frustrated Ferromagnets
11:40	12:00	**J. Schliemann:** Noncollinear ferromagnetism in (III,Mn)V semicondutors
12:00	12:20	**I.A. Abrikosov:** Electronic structure, magnetic, and thermodynamic properties of TM impurities in GaAs
12:20	14:00	Lunch

Magnetotransport + Magnetooptics

14:00	14:30	**B.L. Gallagher:** Magneto-transport properties of high quality ferromagnetic $Ga_{1-x}Mn_xAs$
14:30	15:00	**S. Das Sarma:** How to make semiconductors ferromagnetic: A first course in spintronics
15:00	15:30	**T. Jungwirth:** Theory of magneto-transport properties of Mn-doped III-V semiconductors
15:30	16:00	**K. Ando:** Magneto-optical spectroscopy of DMS with ferromagnetism
16:00	16:20	**J. Sinova:** Magneto-optical properties of metallic (III,Mn)V magnetic semiconductors
16:20	16:50	Coffee Break
16:50	18:30	**Discussion Period**

Saturday, June 14

Collective Excitations

9:00	9:30	**J.K. Furdyna:** Ferromagnetic resonance in $Ga_{1-x}Mn_xAs$
9:30	10:00	**M. Potemski:** Electronic transport and spin excitations in n-type DMS quantum wells
10:00	10:30	**W. König:** Collective spin excitations in DMS Bulk and Quantum-Well Systems
10:30	11:00	Coffee Break

Magnetism of DMS

11:00	11:30	**H. Katayama-Yoshida:** Magnetic Mechanisms and Materials Design of DMS from First Principles
11:30	11:50	**S. Sanvito:** Are (Ga,Mn)As and (Ga,Mn)N really different?
11:50	12:10	**S. Picozzi:** Mn-doped group IV semiconductors: structural and chemical effects
12:10	12:30	**G. Bouzerar:** Disorder effects in DMS
12:30	14:00	Lunch
14:00	15:00	**T. Dietl:**Theories of hole-mediated ferromagnetisms *vis à vis* experimental results
15:00	...	Group discussions

Abstracts

Overview

Theory of Magnetic Semiconductors

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This workshop grew out of a conversation during a Gordon Research Conference on Magnetism about the relationship between first principles and phenomenological theories of ferromagnetism in diluted magnetic semiconductors, especially (III,V) semiconductors containing Mn. Even since that relatively recent conversation, considerable progress has been made in manipulating DMS materials, in measuring the dependence of their properties on growth and annealing protocols, and in understanding the ranges of validity of different theoretical approaches and approximation schemes. In this talk I will attempt to summarize some of what is known about these materials and to frame questions on which progress can be made during the workshop.

any models of (III,Mn)V ferromagnetism assume from the beginning a model in which the important degrees of freedom are the orientations of S=5/2 Mn ion spins and holes in the semiconductor valence band. I will discuss experimental evidence in favor of this assumption and also comment on how this property would be reflected in the quasiparticle bands that emerge from different electronic structure calculation schemes. Given this vastly simplifying assumption, there is still the question of determining the effective Hamiltonian that determines the model's quantum dynamics and low-energy magnetic and transport properties. I will discuss a practical approximate recipe with no free parameters which can be used to model DMS ferromagnetism, and address the possibility of improving on this recipe by using information extracted from first-principles theory and from experiment. One important conclusion that follows from this model is that spin-orbit interactions play an essential role in determining many properties of these unusual ferromagnets, in particular in increasing the magnetic stiffness and thereby ensuring the approximate validity of mean-field-theory approaches. Finally, I will discuss the important role of the disorder that is always present in these materials, emphasizing the advantages of generalized coherent-potential-approximation schemes when disorder is strong and the necessity of accounting for long-range Coulomb scattering in any quantitative model.

Exchange interactions and residual resistivity in DMS from first principles

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[2]*Institute of Physics AS CR, Prague, Czech Rep.*

The talk reviews an ab initio approach to determine thermodynamic and transport properties of diluted magnetic semiconductors (DMS). The approach is based on selfconsistent electronic

structure calculations within the local spin-density approximation (LSDA) and the tight-binding linear muffin-tin orbital (TB-LMTO) method. The substitutional randomness inherent to the DMSs is treated in the coherent potential approximation (CPA). The exchange interactions are studied in the framework of an effective classical Heisenberg Hamiltonian, the parameters of which are determined using the magnetic-force theorem. They are employed in subsequent evaluation of magnon spectra, the spin-wave stiffness constants and the Curie temperatures. The transport properties are investigated within the Kubo-Greenwood linear response theory.

Examples of applications include selected group-IV and III-V based DMSs like, e.g., (Ga,Mn)As, GeMn, with particular attention focused on the role of native compensating defects (As-antisites, Mn-interstitials) as well as of the local moment disorder of Mn atoms.

Defect-Controlled Magnetism in the Ferromagnetic Semiconductor (Ga,Mn)As

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We have studied the magnetic and transport properties of the ferromagnetic semiconductor (Ga,Mn)As as a function of both annealing time and Mn concentration. Annealing at a relatively low temperature (250 degrees Celsius) for less than 2 hours significantly enhances the conductivity and ferromagnetism, but continuing the annealing for longer times suppresses both. These data indicate that such annealing induces the defects in (Ga,Mn)As to evolve through at least two different processes. We have also studied a series of samples grown with Mn concentration between 1.35temperature, conductivity, and exchange energy increase with Mn concentration up to 5concentrations. The ferromagnetic moment per Mn ion decreases monotonically with increasing Mn content, implying that an increasing fraction of the Mn spins do not participate in the ferromagnetism. The data also indicate that, in addition to the carrier concentration, the sample thickness limits the maximum attainable ferromagnetic transition temperature in this material - suggesting that the free surface of (Ga,Mn)As epilayers is important in determining their physical properties. Most recently, we have obtained transition temperatures up to 150 K by annealing 15 nm thick epilayers with high Mn concentration which were grown with a relatively low Ga:As beam equivalent pressure ratio. The combination of all these data suggests that a complex interplay between different defects controls the magnetic properties in this material.

Research has been supported by DARPA and NSF

*In collaboration with: S. J. Potashnik, K. C. Ku, M. B. Stone, S. H. Chun, J. J. Berry, R. Mahendiran, R. F. Wang, and N. Samarth.

Mechanism

Role of Defects in DMS Alloys

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The two most widely studied types of DMS compounds are the group n- and Cr-doped III-V compounds and Co:TiO_2. Of the former, Mn:GaAs is the best studied. In that case, it has long been known that the Mn acceptors are heavily compensated. There is a growing consensus that Mn interstitials and As antisite defects are both present in large numbers, though how many defects are present of each type is somewhat controversial.

Here we consider the effect of both kinds of defects on the magnetic exchange interactions. Both defects compensate the Mn acceptors, reducing T_c, but the Mn interstitial have an added effect of contributing an (antiferromagnetic) exchange interaction that partially compensates the loss of exchange coupling from compensation.

We investigate exchange interactions and magnetic properties using a first-principles LDA method. Using quasirandom structures of large supercells, representative random alloys of varying concentrations were constructed. Also considered were δ-doped structures. Using a linear-response technique, the LSDA total energy is mapped analytically onto a magnetic hamiltonian for both kinds of structures. Temperature-dependent properties, including T_c, are computed from spin-dynamical simulations. It is found that the mean-field estimates of T_c are much too large in these disordered alloys. Based on the T_c computed for compensated alloys, we argued that a significant fraction of the compensators must be Mn interstitials in order for T_c to correspond to experiment.

Using a similar approach, The electronic structure of TM-doped TiO_2 is investigated. We show that in order to explain the observed n type behavior, the Co substitutional dopants must be heavily compensated by a shallow donor, most likely O vacancies or Co interstitials. In either case, T_c that results is far lower than the above RT values observed experimentally, at the concentrations reported. Therefore, we conclude that the magnetism in Co:TiO_2 comes from a distinct phase.

Exchange interactions and Curie temperatures in diluted magnetic semiconductors

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[2]*ISIR, Osaka Univ., Osaka 567-0047, Japan*
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The ferromagnetism in diluted magnetic semiconductors (DMS) has been investigated theoretically either by a model Hamiltonian or by ab initio methods. Despite of their basic differences,

both methods gave similar predictions for the ferromagnetism. Nevertheless, no consensus has been reached about the origin of the ferromagnetism. In fact, Dietl et al. proposed Zener's p-d exchange interaction to describe ferromagnetic DMS [1], on the other hand, Akai pointed out that the double exchange mechanism is responsible for the ferromagnetism [2]. In this paper, we would like to show that both mechanisms are important for understanding ferromagnetism in DMS based on ab initio calculations for Mn-doped III-V compounds. The calculations use the Korringa-Kohn-Rostoker coherent-potential-approximation (KKR-CPA) method to describe the substitutional and magnetic disorder. By mapping the total energy results on a Heisenberg model, the Curie temperature Tc is estimated in the mean field approximation. It is found that if impurity bands are formed in the gap, as it is the case for (Ga, Mn)N, double exchange dominates leading to a characteristic $c^{(1/2)}$ dependence of Tc as a function of the Mn concentration c. On the other hand, if the d-states are localized, as in (Ga, Mn)Sb, Zener?s p-d exchange prevails resulting in a linear c-dependence of Tc. (Ga, Mn)As is an intermediate case, showing a $c^{(1/2)}$ like behavior in the local density approximation (LDA), but a nearly linear c-dependence, if the LDA+U method, with U=4eV, is used.

[1] T. Dietl, H. Ohno, F. Matsukura, J. Cibert and D. Ferrand, Science 287 (2000) 1019.

[2] H. Akai, Phys. Rev. Lett. 81 (1998) 3002.

Mn impurities in III-V semiconductors: from shallow to deep levels

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G. M. Stocks[2] and W. H. Butler[3]

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Mn impurities in Ga based III-V semiconductors acquire either a divalent or trivalent configuration. Simple models that are based on experimental observations assume that Mn in GaAs is in a d^5 configuration with a delocalized hole in the As p-band. Mn in GaN is found to be in a d^4 configuration but the situation in GaP is still under debate. In the present work we have performed ab-initio calculations of the valency of a substitutional Mn impurity in GaN, GaP, and GaAs. We use the self-interaction corrected local spin density (SIC-LSD) method which is able to treat localized impurity orbitals properly. For Mn in GaAs we find that all five majority d-orbitals are filled with one hole in the majority valence band. The magnetization profile shows substantial polarization on the As sites that is anti aligned with the Mn moment and extends over several shell. Magnetic coupling is thus possible between distant Mn neighbors. These results are consistent with the $(d^5 + h)$ model that is stipulated by experiment. When Mn is introduced in GaN, only four d-orbitals are filled. In this case the induced polarization is short ranged and aligned with the Mn moment. The valency of Mn in GaP is similar to that of Mn in GaN. However, the induced magnetization in the hosts shows a mixture of the two respective scenarios found in GaAs and GaN. Work supported by the Defense Advanced Research Agency and by DEO Office of Science through ASCR/MICS and BES/DMSE under

Contract No. DE-AC05-00OR22725 with UT-Battelle LLC.

Material Comparisons

Tight-binding theory for diluted ferromagnetic semiconductors

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An introduction to Slater-Koster tight-binding theory for diluted ferromagnetic III-V semiconductors is given. This theory can serve as a bridge between ab-initio calculations and model descriptions in that it combines a realistic band structure with the possibility to apply many-body techniques, e.g., to treat correlations. As one application, an improved theory for the hole-manganese spin exchange interaction in (Ga,Mn)As is presented. Also, the spin-resolved density of states and projected d-orbital density of states for (Ga,Mn)As are calculated and discussed as functions of d-orbital energy and Coulomb-interaction strength.

Electronic and magnetic properties of GaMnAs alloys: ab-initio LDA+U study

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The study of diluted magnetic semiconductors (DMS) represents a challenge for ab-initio theory because the validity of the local density approximation (LDA) is questioned for such materials. We present a systematic comparative study of the electronic, magnetic, and temperature-dependent properties of (Ga,Mn)As alloys without as well as with As-antisites in the framework of the LDA and LDA+U approaches. The LDA+U is the simplest yet accurate approach to account for electronic correlations beyond the LDA. We apply here the LDA+U approach to random Mn-atoms while remaining atoms are treated in the LDA. The disorder in the system is included in the framework of the coherent potential approaximation. Corresponding temperature-dependent properties, in particular the Curie temperature, are obtained by mapping of the calculated total energies onto the effective classical Heisenberg Hamiltonian and by its statistical study, presently in the framework of the mean-field approximation.

Results indicate a significant weakening of Mn-related features at the Fermi energy and an increase of the local Mn-magnetic moment as compared to the LDA. We will also discuss the results of the dependence of effective pair interactions on the distance and Curie temperatures on the alloy composition in both LDA and LDA+U approaches.

(*) In collaboration with I. Turek, V. Drchal, P. Weinberger, and P. Bruno

Mn doped diluted magnetic semiconductors - a comparative study

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Diluted magnetic semiconductors (DMS) are considered to be vital ingredients in present and future spintronics applications. III-V semiconductors doped with 3d transition metals especially Mn, are the mostly studied materials nowadays. We will present ab-initio electronic structure calculations of Mn doped semiconductors. Results for a comparative study of n doping in III-V, II-VI and Gr. IV semiconductor host will be shown. A special emphasis will be given on Mn doped GaN system as it shows different behaviour compared to a Mn doped GaAs system. Magnetic interactions in presence of interstitial Mn atom acting as self-compensating defect will be discussed. Lastly, we will present effects of strong correlations in Mn doped DMSs studied by LDA+U method.

Half-metallic Zinc-blende Compounds and Multilayers with Semiconductors

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Zinc-blende compounds of transition elements with group-V and VI elements, such as CrAs, have been reported to be half-metallic with high Curie temperature. They represent the concentrated limit of magnetic semiconductors. The fabrication of such materials and their multilayers with semiconductors has also been reported [1] In a recent paper [2] we made an extensive theoretical study of the bulk of such materials and found that the half-metallic property depends on the lattice constant. We have identified systems which have equilibrium lattice constants close to the ones of semiconductors, and which are also half-metallic in these lattice constants. In this way we propose possible half-metal semiconductor combinations for coherent growth with small lattice mismatch. These are VAs/GaAs, VSb/InAs, VSb/GaSb, CrAs/GaAs, CrSb/InAs, CrSb/GaSb, MnSb/GaSb. We also extend our calculations to the case of the (001) multilayers CrAs/GaAs, CrSb/InAs, CrAs/ZnSe and CrSb/ZnTe. We find that half-metallicity can be preserved throughout the multilayers.

1. H. Akinaga *et al.*, Jpn. J. Appl. Phys. **39**, L1118 (2000); M. Mizuguchi *et al.*, J. Magn. Magn. Mater. **239**, 269 (2002).

2. I. Galanakis and Ph. Mavropoulos, Phys. Rev. B **67**, 104417 (2003).

Control on hyperfine interactions of antisite As in $(In_{1-x-y}Mn_xAs_y)As/AlAs$ through bias voltages

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Recent developments in fabrication of diluted magnetic semiconductors (DMS) have realized ferromagnetic quantum superstructures using DMS's, typically (Ga, Mn)As and (In, Mn)As. This opens up the possibility that the hyperfine fields seen by the nuclei in these systems are tailored by adjusting the band alignment, doping, and bias voltage. Such techniques are necessary to manipulate nuclear spins in, for instance, quantum computers using nuclear spins. They can be also very important in determining nuclear parameters such as nuclear magnetic-dipole and electric-quadrupole moments. In this paper we propose a new method of controlling hyperfine interactions by use of hetero structures of DMS's. Due to the s-d hybridization the s state of the constituent atoms is exchange split, which produces non-zero hyperfine field on the nuclei through Fermi's contact interaction between the electron spin and nuclear spin. In certain situations, this contact interaction becomes rather sensitive to the bias voltage at the interface. As an example, we show the results of the first-principles calculation on the bias dependency of the magnetic hyperfine field at the anti-site As in $(In_{1-x-y}Mn_xAs_y)As/AlAs$. The calculation is based on the local density approximation and the KKR-CPA (Green's function method combined with the coherent potential approximation) which properly takes account of the random substitution of In atoms for Mn and anti-site As atoms. The bias voltage is applied between $(In_{1-x-y}Mn_xAs_y)As$ and AlAs and the contact hyperfine interaction, which in a non-relativistic approximation is proportional to the magnetization produced by the electron spins at the nuclear position, for each component atom is calculated. The hyperfine fields at In and Mn atoms turn out not to be very sensitive to the bias voltage. However, the hyperfine field of the anti-site As strongly depends on the bias voltage: The hyperfine filed changes from nearly zero to -60 T when the bias voltage varies from zero to -0.5 V. The underlying mechanism of this bias dependence of the hyperfine field is well explained in term of the local electronic structure. The results of calculation on several other superstructures of DMS's are also presented.

Spin Injection

Spintronic Nanostructures

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Semiconductor spintronics has now reached a stage where the basic physical mechanisms controlling spin injection and detection are understood. At the same time, some of the critical technological issues involved in the growth and lithography of the magnetic semiconductors have been solved.
Together, these development allow the experimentalist to explore the physics of spintronic nanostructures. In this contribution, I will discuss some of our recent research in this direction. Specifically, I will address magnetic resonant tunneling diodes that can be operated as a voltage controlled spin-switch, as well the observation of a very large spin valve effect occurring at sub-10 nm sized constrictions in a ferromagnetic semiconductor.

Spin Polarized Electron Injection from Ferromagnetic Semiconductors and

Metals

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Electrical injection, transport and manipulation of spin polarized carriers in a semiconductor are essential requirements for utilizing the spin degree of freedom in a future semiconductor spintronics technology. Ferromagnetic semiconductors (FMSs) are promising candidates in this effort - their exchange split band edges offer both spin injection and spin-selective transport in heterostructures. An n-type FMS is especially attractive, since electron transport is the basis for high frequency, low power operation. Recent work demonstrated epitaxial growth of n-type CdCr2Se4, a chalcogenide spinel FMS, on GaAs(001) and GaP(001) [1]. We report here measurements of electrical spin injection, band offsets, and interface structure in CdCr2Se4/ AlGaAs/ GaAs structures. Band gap engineering enables spin injection into the GaAs quantum well (QW), where the selection rules governing radiative recombination provide a direct link between the measured circular polarization and the electron spin population. Ferromagnetic metals are also attractive as spin injecting contacts because they offer a source of spin polarized electrons, high Curie temperatures, low coercive fields and fast switching times. We have successfully injected polarized electrons from an Fe contact into an AlGaAs/GaAs LED and obtained electron spin polarizations of 13% in the GaAs QW [2]. We report here very recent efforts to improve the structure, resulting in an increase of electron spin polarization Pspin = 32% in the (001) QW. We demonstrate via the Rowell criteria that tunneling is indeed the dominant transport process, and confirm that majority spin electrons are responsible. TEM shows that the interface is well-ordered and epitaxial. Preliminary results for spin injection into a GaAs(110) QW are also presented.

This work was supported by the DARPA SpinS program (S. Wolf) and ONR (L. Cooper).

[1] Y.D. Park, A.T. Hanbicki, J.E. Mattson and B.T. Jonker, APL 81, 1471 (2002).

[2] A.T. Hanbicki, B.T. Jonker, G. Itskos, G. Kioseoglou and A. Petrou, APL 80, 1240 (2002); cond-mat/0302221.

A challenge for spintronics: spin injection into semiconductors (theory and experiments)

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I will report on theory and experiments of spin injection into semiconduc-tors and the ability to detect electrically the induced spin-polarization. Ex-periments consists in injecting spins into a

p-type GaAs quantum well from a ferromagnetic emitter of GaMnAs through an AlAs barrier. The spin detec-tion is performed electrically by probing how the current, tunneling towards a GaMnAs collector through a second AlAs barrier, depends on the orientation of its magnetization. The structures we study are double barrier junctions of the type GaMnAs/AlAs/GaAs(3, 6, 9nm)/AlAs/GaMnAs elaborated by molecu-lar beam epitaxy at low temperature. The existence of large TMR ratio ap-proaching 40% at lowest temperature (4K) for double junctions with a non-magnetic central layer is a new and interesting effect, never observed in metallic double junctions[1]. We discuss the conditions to observe such magnetoresis-tance effects by comparing the carrier lifetime in the well to the spin lifetime. Results we observe lead to an estimate of the hole spin lifetime in the nanosec-ond range at 4K in agreement with previous dynamical optical measurements[2]. Moreover, I will show that the variation of the magnetoresistance with tempera-ture constitutes a probe for the measurement of the spin lifetime in semiconduc-tor nanostructures. To conclude, I will show that our results can be equivalently accounted in term of sequential tunneling without spin relaxation that is spin accumulation in the GaAs well[3] like appearing in the treatment of CPP-GMR for metallic multilayers.

[1] R. Mattana et al., cond-mat/0211409, to appear in Phys. Rev. Lett. (05/2002).

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Spin coherence and dephasing of donor and free band electron spins in n-GaAs across the metal-insulator transition

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The fundamental physical processes responsible for the long spin lifetimes exceeding 100 ns in n-GaAs [1] are not well understood. To identify the relevant electronic states and to understand the underlying spin dephasing mechanisms, we performed time-resolved magneto-optical Kerr spectroscopy on Si doped GaAs for concentrations ranging from 2×10^{15} to $2 \times 10^{18}/rmcm^3$. By varying the photon energy both free band electron spins at higher energies and donor spins at lower energies can optically be excited. A separation of both contributions is feasible according to their distinct spin lifetimes, electron g-factors, and doping concentration across the metal-insulator transition (MIT). The longest spin lifetimes (¿100ns) can be assigned to the donor-related electronic states, which show the strongest B-field dependence. Free band electron spins have significantly shorter spin lifetimes depending less on B-field. The results suggest that the spin dephasing mechanisms for the donor related electron spins strongly depend on the carrier localization length, which diverges at the MIT.

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Defects and Magnetism

Tale of Two Sites: Substitutional vs. interstitial doping in DMS

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Substitutional doping by magnetic ions is the basis for ferromagnetism in many dilute magnetic semiconductor systems. Typically, the substitutional dopant acts as an acceptor, leading to a kinetic-exchange interaction that produces a ferromagnetic ground state. The situation is very different when dopants occupy interstitial sites, where they typically (but not always) act as donors and thus suppress the ferromagnetic interaction. This talk will describe three DMS systems in which interstitials play an important role: Mn-doped GaAs, Co-doped TiO2 anatase, and (hypothetical) Mn-doped diamond.

Incorporation of Mn atoms into diluted magnetic semiconductors

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We examine the energetics of diluted ferromagnetic III-V semiconductors on an ab initio level using the tight-binding linear muffin-tin orbital method combined with the coherent-potential approximation. Magnetic disorder is treated within the disordered local moment model. Based on total energies and effective interatomic interactions calculated within the generalized perturbation method, we analyze the local environment effects on formation energies of antisite defects and substitutional and interstitial Mn atoms. The theory is illustrated on the $Ga_{1-x}Mn_xAs$ alloy system.

Compositional dependence of lattice constant and impurity formation energies in (Ga,Mn)As

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We investigate the compositional dependence of the total energy in mixed (Ga,Mn)Ga crystals containing various native defects and dopants. Combining the density-functional method with coherent-potential approximation we are able to change the chemical composition gradually to perform a detailed scan of the low-concentration range.

Minizing the total energy with respect to the atomic volume, we first show that - in contrast to the general opinion - the lattice constant, a, of a perfect mixed crystals (Ga,Mn)As does

not depend much on the concentration of Mn [1]. On the other hand, a increases linearly with increasing number of Mn atoms that occupy interstitial [2,3,4] instead of substitutional positions. The same happens if As antisite defects are present. As long as these two defects are the most important compensating donors in (Ga,Mn)As, the increase of a is correlated with the degree of compensation, i.e., with the quality of the material. The observed compositional dependence of the lattice constant of (Ga,Mn)As indicates that the number of compensating defects increases proportionally to the concentration of Mn. The comparison with calculated dependence shows an almost complete compensation.

Using a simple relation between the formation energy of an impurity and cohesion energy of the impure crystal [5] we also show that the formation energy of both interstitial Mn and antisite As decreases substantially with increasing concentration of Mn. At the same time, the formation energy for the substitution of Mn decreases in presence of these two donors. This may be an explanation for the above-mentioned self-compensating behavior of (Ga,Mn)As.

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Electronic structure, exchange interactions and Curie temperature in III-V and II-VI DMS

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In this talk I will present the results of the study of (GaT)As [1,2] and (ZnT)Se [3] (T=Cr,Mn,Fe). Also the results of the recent studies of (GaMn)N will be discussed. The calculations are performed in the super-cell approach with the use of helical magnetic configurations for estimation of the interatomic exchange parameters. I will show that this calculational approach provides good description of magnetism of very different DMS systems.

Among others the following issues will be addressed: p-d exchange and giant Zeeman splitting, the role of charge carriers in mediating ferromagnetism, the localization of the carriers, the interplay between the antiferromagnetic superexchange and ferromagnetic kinetic exchange, ferromagnetic exchange path, different role of the As-antisites in different systems.

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Magnetic and Electronic Structure Of $(Ga_{1-x}Mn_x)As$

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We present theoretical calculations of the magnetic and electronic structure of Mn doped GaAs (in the zincblende structure). The magnetic properties are shown to be very sensitive to structural defects, in particular As antisite defects and Mn at interstitial positions. Only when considering such defects can the experimental magnetic moments be reproduced by the first principles theory [1]. We present a simple model for how one can understand the connection between the magnetic ordering and the As antisites, and how the defects help to stabilize a partial disordered local moment (DLM) state. The connection between the energetics of the Mn substitution and the As antisite concentration is also analysed. We also compare the calculated magnetic properties and electronic structures of Mn situated on substitutional sites (Mn replacing a Ga atom) and on interstitial sites, where in agreement with observations the interstitial site is found to be less favourable. oreover, combining our first principles calculations of the spin-wave excitation energies with a classical Heisenberg Hamiltonian we have calculated interatomic exchange interactions and using Monte Carlo simulations we present theoretical values of the critical temperature as a function of Mn concentration for a number of diluted magnetic semiconductor systems [2].

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Disorder and Frustration

Heisenberg-Like Hamiltonian for GaMnAs

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The experimental study of the ferromagnetic moment per Mn ion in post annealed GaMnAs samples shows that a large fraction of the n spins do not participate in the ferromagnetism. It is important to know if the lack of magnetization saturation is due to an extrinsic effect as for example the *wrong* location of the Mn ions in the host semiconductor or it is due to an intrinsic effect related to the spatial oscillatory behavior of the hole mediated interaction between the Mn spins. The study of the last possibility is the main motivation for this work.

The mean field calculations replace the Mn ions by an uniform magnetic field acting on the hole spins. This approach always predicts a full saturated ferromagnetic ground sates for the Mn

spins. It is necessary to introduce thermal fluctuations and disorder in order to study the real ground state of the system. However, as the internal energy in this problem is the kinetic energy of the carriers, standard Monte Carlo simulations are limited to the study of simple electronic models and small systems.

In this work I propose a Heisenberg like Hamiltonian for studying the effect of disorder and thermal fluctuations on the Curie temperature of GaMnAs. The coupling constants of this Hamiltonian are obtained from a realistic six band $\mathbf{k} \cdot \mathbf{p}$ model.

In the talk first I justify the use of this approach, in particular I study: i) the validity of assuming that the interaction between two Mn spins is proportional to their scalar product, ii)the spin anisotropy in the interactions, iii) the spatial anisotropy in the interactions, and iv) the description of the total interaction energy as a sum of pair interactions.

Once the model is justified, I will show Monte Carlo simulations results. From the simulations we analyze the dependence of the Curie temperature on: i) the use of parabolic two or four band models versus the use of more realistic six band $\mathbf{k}\cdot\mathbf{p}$ model, ii)the density of holes, iii)the strength of the exchange coupling and iv) the spatial extension of the exchange interaction between the Mn spins and the holes spins.

Finally, by calculating the coupling constants of the Heisenberg-like model at the zero temperature spin polarization of the carriers, and treating the Mn spin as quantum objects, I obtain the collective excitations of the system. From the low energy excitations I analyze the stability of the zero temperature ferromagnetic ground state.

Magnetic Semiconductors: Frustrated Ferromagnets

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Starting from a microscopic description of the exchange interaction, we derive the effective Mn-Mn interaction in metallic $Ga_{1-x}Mn_xAs$. Due to the strong spin-orbit coupling in the valence band, this effective interaction is highly anisotropic and has a spatial structure somewhat similar to dipolar interactions [G. Zarand and Boldizsar Janko, Phys. Rev. Lett. 89, 047201 (2002)]. The corresponding ground state has a finite magnetization but is intrinsically spin-disordered even at zero temperature, explaining many features of the experimental data. We also derive an effective Hamiltonian for $Ga_{1-x}Mn_xAs$ in the very dilute limit and compute its parameters using microscopic modeling [G. Fiete, G. Zarand, and K. Damle, cond-mat/0212074]: There

$Ga_{1-x}Mn_xAs$ can be described in terms of spin 3/2 bound holes that hop beween the Mn sites with a spin-dependent hopping and couple to the core Mn spins through a local exchange interaction. We find in this model a localization transition, and strong anisotropy disorder, very similar to the one found in the metallic limit. We also find that . upon relaxation - the Mn ions form a regular BCC lattice with some interstitials. Our results are relevant for other p-doped magnetic semiconductors too.

Noncollinear ferromagnetism in (III,Mn)V semicondutors

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We study the ground state properties of kinetic-exchange models for (III,Mn)V semiconductors with randomly distributed Mn ions. Our method is embedded in a path integral spin-wave type formalism leading to an effective action for Mn spins only with full atsubara frequency dependence. The zero-frequency contribution to this action is equivalent to static perturbation theory and characterizes the stability of a given spin configuration, while the component linear in frequency can be interpreted as the joint Berry phase of the Mn and carrier system.
For simple parabolic-band carriers the collinear ferromagnetic state with all Mn spins in parallel is always *stationary* but generically *unstable*. This instability can be characterized in terms of inverse participation ratios and is due to long-ranged nonlocal spin fluctuations. We also present results for the ground state magnetization as a function of an external field.
For carrier dispersions involving anisotropy induced by spin-orbit coupling the collinear state is not even stationary and therefore also not the ground state. This interplay between the anisotropy in the carrier system and the disorder in the Mn positions reflects recent findings by Zarand and Janko [3] obtained within the RKKY approximation.
The stationarity of the collinear state (with the magnetization pointing in one of the cubic symmetry directions) is restored in the continuum or *virtual crystal* approximation where disorder is neglected.

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Electronic structure, magnetic, and thermodynamic properties of transition metal impurities in GaAs

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Electronic structure, magnetic, and thermodynamic properties of 3d- transition metal (TM) impurities, intrinsic point defects, and various defect pairs in GaAs have been studied from the first-principles by means of the coherent potential approximation (CPA) and the locally self-consistend Green's function (LSGF) method. We show that magnetic structures involving disordered local magnetic moments on the Mn atoms in $(Ga_{1-x}Mn_x)As$ lowers the total energy compared to pure ferromagnetic ordering when As defects on the Ga sublattice are considered. Hence a magnetic structure with partial disorder of local moments is demonstrated to be stable for a range of concentrations of As antisites. Only by considering this magnetic configuration can one explain the observed magnetic moments in $(Ga_{1-x}Mn_x)As$. We propose a mechanism for the stabilization of the magnetic structures and conclude that the magnetization and critical temperatures should increase substantially by reducing the number of As antisite defects. Thermodynamics of the point defects is also investigated. Antisite defects, As_{Ga}, are found to be the most energetically favorable defects in the As-rich GaAs. The studied TM-impurities (V, Cr, Mn, and Fe) are found to form substitutional alloys on the Ga sublattice. Thermodynamic possibility of formation of complexes between TM-atoms is investigated.

Magnetotransport and Magnetooptics

Magneto-transport properties of high quality ferromagnetic $Ga_{1-x}Mn_xAs$

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We present a systematic study of magnetotransport in high quality MBE grown and post annealed $Ga_{1-x}Mn_xAs$ (1%¡x¡9%) epilayers. These samples have very high Curie temperatures (up to 159K) and conductivities and very weak isotropic magneto-resistance. This enables us to separate the normal and anomalous contributions to the Hall effect, and so extract reliable hole densities across the range of Mn concentrations. The compensation is found to be very low for the highest Curie temperature samples. We also present accurate measurements of the anisotropic magnetoresistance AMR. The magnitude of the AMR is found to increase with deceasing Mn concentration, reaching 30

The measured Curie temperatures are shown to be in reasonable agreement with the predictions of the mean field theory. The Hall effect and AMR data are found to be in good agreement with theoretical results for a model of band-hole quasiparticles with a finite spectral width due to elastic scattering from Mn and compensating defects.

How to make semiconductors ferromagnetic: A first course in spintronics

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A potentially important recent experimental discovery is that a large number of semiconductors become ferromagnetic when doped carefully with 1-10% of magnetic impurities (mostly Mn although Co has been used in some cases too). Some examples of such 'diluted magnetic semiconductors' (DMS) are GaMnAs, InMnAs, GaMnN, GaMnP, GeMn-there is recent speculation that even the reported ferromagnetism in hexaborides is due to unintentional doping by Fe impurities. Ferromagnetic semiconductors, where magnetic and semiconducting properties can be controlled and tuned at will, are projected to form the basic ingredients in the emerging field of spintronics. I will critically discuss in this talk the physical mechanisms underlying DMS ferromagnetism within a minimal model where magnetic coupling between the impurity local moments is mediated by the semiconductor carriers (mostly valence band holes). Ferromagnetism occurs irrespective of whether the system is metallic or insulating, leading to our recent polaron percolation theory of DMS ferromagnetism. I will discuss the very unusual concave magnetization and related strange behavior shown by DMS systems using a two-component mean field theory, the dynamical mean field theory, and the polaron percolation theory. Extensive comparison between theory and experiment will be presented. The talk will be based on our recent work as appearing in PRL 87, 227202 (2001); PRL 88, 247202 (2002); cond-mat/0211496, and more recent unpublished work.

Theory of magneto-transport properties of Mn-doped III-V semiconductors

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The basic microscopic origins of ferromagnetism in the (III,Mn)As and (III,Mn)Sb compounds appear to be well understood within a model of carrier induced magnetic interactions between Mn local moments. Efficient computation methods have been developed, based on the effective Hamiltonian description of the system, which are able to model their magnetic, transport, and optical properties on a quantitative level. In this presentation we focus on theoretical predictions of the dc- and ac-transport coefficients and make a comparison to the experimantally observed anisotropic magnetoresistance effects and the anomalous Hall effect. We also discuss a microscopic theory of the Gilbert damping of magnetization precession and the spin-transfer process in diluted magnetic semiconductor heterostructures.

Magneto-optical spectroscopy of diluted magnetic semiconductors with ferromagnetism

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Carrier-spin ($s, p-d$) exchange interactions is the most distinguishing character of diluted magnetic semiconductors (DMSs). Magnetic circular dichroism (MCD) spectroscopy is a powerful tool to study the $s, p-d$ exchange interactions in DMSs because MCD sensitively detects the spin-polarized modification of the band structures. In this talk, we discuss the MCD spectra of some of new DMSs.

$In_{1-x}Mn_xAs$[1], $Ga_{1-x}Mn_xAs$[2], and $Zn_{1-x}Cr_xTe$[3] show large MCD signals around the critical point (CP) energies. MCD intensity shows clear ferromagnetic field dependence. Therefore we can conclude that the observed ferromagnetisms arise from DMSs, not from precipitates. $Zn_{1-x}Cr_xTe$ has a high Tc of 300K.

Large MCD signals were also observed in paramagnetic $Zn_{1-x}TM_xO$ (TM = Mn ,Fe, Co, Ni, Cu) [4]. Some ZnO:Co samples showed ferromagnetism. But CD analyses clarified that both of paramagnetic $Zn_{1-x}Co_xO$ and an unidentified ferromagnetic material were contained in the sample [5]. ZnO:Ni [5], GaN:Mn [6], and GaAs:Cr [7] showed only paramagnetic MCD signal.

CD spectral shapes of $Ga_{1-x}Mn_xAs$, $In_{1-x}Mn_xAs$ and $Zn_{1-x}Cr_xTe$ at their Λ-CPs can be qualitatively explained by simple $s, p-d$ exchange interaction induced Zeeman-splittings of their host band structures. On the contrary, the MCD structures around the band-gap energies cannot be explained by a simple model of Zeeman-splittings of the host band structures. Even their polarities are opposite to the expected ones. We guess that these anomalies around E_g arise from the strong mixing of the d-orbital with the valence bands of the host semiconductors. The analyses of the MCD spectral shapes of the ferromagnetic DMSs have been done only qualitatively. Quantitative comparisons with theoretical calculations are desired.

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Magneto-optical properties of metallic (III,Mn)V magnetic semiconductors

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etallic diluted magnetic semiconductors materials offer a much wider spectrum of magneto-transport and magneto-optic effects than conventional itinerant electron ferromagnets, mostly due to the greater tunnability of the Mn moments ordered state through growth conditions, doping, gates, and light. Here we study the infrared magneto-optical properties of metallic (III,Mn)V semiconductors based on the itinerant hole-fluid model. Within this approach we consider the virtual crystal approximation, applicable to the cleaner metallic samples, including disorder scattering within a Bohrn type approximation, and a finite size self-consistent calculation where disorder and interactions are treated in an equal footing. We will discuss the different results and predictions of these calculations and its agreement to experiments and demonstrate the possibility of using optical absorption as a tool to measure the itinerant carrier density. We also calculate the Faraday and Kerr effects within the infrared regime and predict a large resonant behavior at intermediate frequencies which should be readily observable in current experimental set ups.

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Collective Excitations

Ferromagnetic resonance in $Ga_{1-x}Mn_xAs$

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We present a systematic study of ferromagnetic resonance carried out on a series of specimens of the ferromagnetic semiconductor $Ga_{1-x}Mn_xAs$ in thin film form. The GaMnAs layers were grown by low-temperature molecular beam epitaxy either on GaAs or on GaInAs buffers, the two buffers being used to obtain different strain conditions within the ferromagnetic layer. Our aim is to map out the dependence of the FMR position on temperature and on the angle between the applied magnetic field and crystallographic axes of the sample. The analysis of the FMR data allows us to obtain the values of the cubic and the uniaxial magnetic anisotropy fields M-(C- i.e., those which are associated with the natural (undistorted) zinc-blende structure, and those arising from of strain. In addition to the main ferromagnetic resonance line that provides information on magnetic anisotropy of the GaMnAs alloy, we will also present experimental data

showing well-resolved spin wave resonances that accompany FMR in the form of satellite peaks; and we will describe systematic trends observed in FMR broadening as a function of temperature and field orientation with respect to the crystallographic axis of the GaMnAs specimen.
In collaboration with X. Liu

Electronic transport and spin excitations in n-type DMS quantum wells

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The experimental studies of a model diluted magnetic semiconductor (DMS) structure, namely very diluted Mn^{2+} ions coupled to an electron gas both of which are confined in a CdMnTe quantum well structure, will be reported. The consequences of the s-d exchange interaction on the transport properties of a 2DEG at low magnetic fields will be shown and the characteristic features of the longitudinal and transverse resistance of a 2DEG at high magnetic fields, when the effective electronic Zeeman splitting vanishes, will be discuss. The investigations of the characteristic spin excitations in these systems, as deduced from Raman scattering experiments as well as from measurements of resistively and optically detected EPR, will be then presented. The observation of the avoided crossing between the characteristic spin excitations of 2D electrons and Mn^{2+} ions, when spin polarization of both subsystems is induced by the application of a magnetic field, will be reported and this effect will be discussed in a view of a possible collective character of spin excitations in n-type DMS semiconductors.

Collective Spin Excitations in Diluted Magnetic Semiconductor Bulk and Quantum-Well Systems

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We present a theory of collective spin excitations in diluted magnetic semiconductors, based on a phenomenological approach of a kinetic-exchange coupling between localized Mn spins and itinerant carrier spins. For p-doped bulk systems we derive spin excitation spectra and discuss the importance of a proper modeling of the band structure by using either a simple two-band [1] or a more advaced six-band [2] Kohn-Luttinger Hamiltonian. We extend our theory for quasi-two-dimensional systems. With this, we can explain [3] the anomalously large Knight shift observed in recent electron-paramagnetic-resonance experiments, and we address the physics of ferromagnetism in n-type diluted magnetic semiconductor quantum-well systems. Furthermore, we analyze [4] the multiplett of spin-wave spectra as a function of carrier concentration.

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Magnetism of DMS

Magnetic Mechanisms and Materials Design of Diluted Magnetic Semiconductors from First Principles

Guideline for high-Tc and application to II-VI, III-V, IV, and I2-VI Semiconductors

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We will discuss the ferromagnetic mechanisms of high Curie temperature (high-Tc) diluted magnetic semiconductors (DMSs) based upon ab initio electronic structure calculations. We found four competitive contributions to the ferromagnetic and anti-ferromagnetic mechanisms in the real DMSs materials; (i) ferromagnetic Zener's double-exchange interaction, gives high-Tc, if anti-bonding ta-impurity d-band is partially occupied by electrons, (ii) ferromagnetic Zener's p-d exchange interaction, gives low-Tc, (iii) Super-exchange interaction (Kanamori-Goodenough rule; occupied ta-impurity band gives anti-ferromagnetic interaction and occupied e-impurity band does ferromagnetic interaction) in compound semiconductors such as GaAs and GaN, and (iv) Direct-exchange interaction (Alexander-Anderson-Moriya interaction; half-filled Cr and Mn are anti-ferromagnetic, and Ti, V, Fe, Co, Ni are ferromagnetic states) in Si and Ge. Based upon these four competitive mechanisms, we propose a new guideline (Katayama-Yoshida rule) for the realization of high-Tc DMSs. Based upon the guideline, we have designed (1) transparent high-Tc half-metallic ferromagnets in 3d-transition atom (TM) doped II-VI (V and Cr) and III-V (V, Cr, and Mn) DMSs, (2) 3d-TM doped IV (Cr and Mn) high-Tc DMSs by choosing inhomogeneous-doping (Zincblende-type atomic-layer epitaxcy [ALE]), (3) Delta-doping by ALE for V-, Cr- and Mn-doped GaAs and GaN, (4) 4d- and 5d-TM doped I2-VI based transparent half-metallic high-Tc DMSs such as K2S and K2Se, and (5) 4f-rare earth atom doped high-Tc Si, GaN and AlN. (5) 3d-TM doped diamond never shows magnetic state due to the too strong p-d hybridization.

Are (Ga,Mn)As and (Ga,Mn)N really different?

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The electronic structures of Mn-doped zincblende GaAs and wurtzite GaN are calculated using both standard local-density functional theory (LSDA), and a novel self-interaction-free approach, able to account for strongly-correlated effects [1]. We find that in (Ga,Mn)As the Fermi energy is crossed by weakly correlated p-d hybridized bands. The Mn 3d character is distributed through the whole valence band manifold, and therefore the self-interaction does not strongly affect the photoemission properties. This validates the extensive literature of LSDA studies of this material, including the conclusion that the ferromagnetism is hole-mediated.

In contrast (Ga,Mn)N is characterized by localized Mn 3d bands and the self-interaction is very strong. Our calculations show a highly confined $d_z{}^2$-p_z hole just above the Fermi energy in the majority band manifold. In this case no holes are left in the GaN valence band and the ferromagnetic coupling is rather short range.

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Mn-doped group IV semiconductors: structural and chemical effects on ferromagnetism

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A review of the results obtained by means of first principles simulations within density functional theory for Mn impurities in a group IV matrix (i.e. Si, Ge and SiGe alloys) will be presented. In particular, we will focus on the structural, electronic and magnetic properties of *i)* n_xGe_{1-x} and Mn_xSi_{1-x} ordered alloys, as a function of the Mn concentration and the spin magnetic alignment (*i.e.* ferromagnetic vs antiferromagnetic), *ii)* Mn:Si_yGe_{1-y} alloys as a function of the host matrix, both within the "real-atoms" and the "virtual crystal" approach, *iii)* [001] ordered $(Mn)_1/(Ge)_n$ digital alloys, as compared with systems where Mn atoms are homogeneously distributed within the Ge host matrix; *iv)* Mn defects in Si as a function of their charge state and position (interstitial - Mn_I-, substitutional - Mn_s-, or Mn_I-Mn_s complexes), in terms of formation energies and magnetic moments. Finally, we will perform a comparison with available photoemission data, showing a good agreement between theoretical and experimental core levels as a function of the chemical environment.

Disorder effects in diluted ferromagnetic semiconductors

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In the first part, we will analyze the effect of disorder in diluted III-V magnetic semiconductors (DMS) on a model level by adopting a two step approach.In the first step, we calculate the element resolved configurationally averaged Green's function of itinerant carriers in the framework of the single-site coherent-potential approaximation (CPA). Then, using a generalized RKKY formula, we evaluate the long-range exchange integrals between magnetic atoms and the corresponding Curie temperature as a function of the exchange parameter strength, the magnetic impurity concentration, and the carrier density. A proper treatment of the disorder which includes all single-site multiple-scattering events appears to play a crucial role. We demonstrate that the standard RKKY calculations, which neglect the effect of disorder, strongly underestimate the Curie temperature and are inappropriate to describe the magnetism in DMS. It is also shown that a local antiferromagnetic exchange favors higher Curie temperature. In the second part, using first principle calculations, we determine the Curie temperature in (Ga,Mn)As alloys. The disorder due to random positions of Mn-impurities and As-antisites is also taken into account in the framework of CPA. We demonstrate that a simple mean-field approximation (MFA) provides already T_c accurately. In particular, it is shown that the calculated T_c in the random-phase approximation and Monte Carlo simulations differ only weakly from the FA values. The reason of the validity of MFA is discussed.

Theories of hole-mediated ferromagnetisms *vis à vis* experimental results

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Despite many years of extensive research the nature of hole-mediated ferromagnetism in tetrahedrally coordinated semiconductors remains controversial. In particular, among other more exotic proposals, double exchange, Zener/RKKY, and polaron mechanisms have been invoked.

A highly subjective survey of relevant experimental findings will be presented, showing that the relevant carriers of magnetic information are delocalized or weakly localized holes in the host valence band. The experiments to be discuss include the Curie temperature, spontaneous

magnetization, magnetic and resistance anisotropy, domain structure, optical properties, and inelastic neutron scattering.

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3 News from the ESF Psi-k Programme

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

3.1 Reports on Collaborative Visits

Report on the visit of Zs. Major (University of Bristol) to Prof. H. Ebert's group (Ludwig-Maximilians-Universität, Munich)

16-20 June 2003

Calculating electron–positron momentum densities within the Munich SPR–KKR program package

During my stay with Prof. Ebert's group in Munich we started on the implementation of electron–positron momentum density calculation within the fully relativistic KKR-CPA framework, as an extension to the SPR–KKR program package.

Calulating the electron–positron momentum density in metals is a very useful tool in conjunction with two-dimensional **A**ngular **C**orrelation of Electron-Positron **A**nnihilation **R**adiation (2D-ACAR) experiments. Here the 3D momentum distribution in a metal is probed by using positrons and a two-dimensional integration of the electron-positron momentum density is obtained. From these data information about the Fermi surface (size and topology) can be extracted. In order to analyse, understand, and interpret these positron data, comparison with electron–positron momentum densities from first–principles calculations is essential.

The SPR–KKR program package already offers the possibility to calculate the electron momentum density and thus Compton profiles, implemented by Prof. Ebert and D. Benea. Together with them we agreed on what differences the presence of the positron will cause and how this can be included in the already established framework of Compton scattering for the most general case (disordered alloy with many atoms per unit cell). We found that under the assumption that there is only one positron present in the system at any given time (which is in agreement with the experimental situation), it is the matrix elements that need to be modified and weights depending on the positron wavefunction will enter the expressions. Preliminary tests showed that by changing the sign of the potential seen by the electron and not taking into account the exchange contribution, the positron potential can be calculated within the SPR–KKR code, and from this the energy and the wavefunction of the positron needed for the matrix elements and weights can be obtained.

We test the electron–positron momentum density code by comparison with results from LMTO calculations. First calculations already showed that the electron momentum density is modified in the 'correct direction' when positron effects in the matrix elements are taken into account, i.e. the contribution in momentum space falls off more rapidly than in the electron momentum density. The remaining step of the implementation is to produce an output which can be compared to 2D-ACAR data, i.e. to perform the integration of the three-dimensional momentum density to get two-dimensional distribution functions. This will be done and tested within the next weeks.

3.2 Reports on ESF Psi-k Workshops

3.2.1 Report on Workshop on "Electronic Transport in Molecular Systems"

CECAM
ESF/Psi-k

Workshop
on

"Electronic Transport in Molecular Systems"

CECAM,
Lyon,
2-5 June 2003

Supported by:

CECAM
ESF/Psi-k

A workshop on the "Electronic Transport in Molecular Systems" was organized by Xavier Blase (Lyon, France), Christophe Delerue (Lille, France) and Kurt Stokbro (Lyngby, Denmark) in CECAM (Lyon) and was attended by 43 participants. It was sponsored by the CECAM and the ESF/Psi-k programs.

The aim of this workshop was to bring together experts with widely different backgrounds to discuss current issues and trends in the modelling of the electronic transport in molecular systems. The various transport formalisms, the influence of electron-electron and electron-phonon interactions on the I/V curves were discussed. Introductory lectures on the experimental aspects of molecular transport and on the physics of mesoscopic systems in general completed the workshop. Under the ESF/Psi-k program, this workshop served as a starting point to a European Working group on Molecular Electronics (WG8).

The scientific background, motivations and objectives of the workshop are listed below.

Scientific background

With the advancement of techniques for characterizing and manipulating individual nano-objects such as molecules, metallic nanowires or nanocrystals, there has been significant progress in the development of nano-electronics and molecular electronics in recent years. Several research groups have reported measurements of electrical transport through single or small groups of molecules. Experimental current-voltage I(V) curves display complex features which arise from the quantum states of the system and from the large perturbation induced by the motion of a single electron into the nanostructure. One critical issue is the interpretation of the experiments which most of the time requires detailed calculations of the transport properties. Predicting the electrical properties of nanostructures theoretically is a very complex problem. Typically, for a molecule between two electrodes, there are many processes involved in the transport: charge transfer between the molecules and the electrodes, interaction of the levels with the continuum states of the electrodes, strong electron-electron interactions, molecular vibrations which may induce inelastic scattering. Another fundamental issue is that the molecular devices are out of equilibrium whereas most of the state-of-the-art electronic structure calculations are presently made for systems at equilibrium. Up to now, computational techniques used to solve these problems have been based on non-selfconsistent Hückel or tight-binding calculations [1-9] which have provided valuable insights into the identification of the conduction mechanisms. Recent works have dealt with first-principles calculations based on the density functional theory, solving the problems self-consistently, which is crucial to determine the level positions with accuracy [11-21]. However, many important questions remain to be solved, such as those concerning the importance of exchange-correlation effects [6,22] and electron-phonon couplings [23-26]. On the computational side, many developments are still necessary, in particular to be able to study the transport through molecules containing a large number of atoms, such as oligomers, nanotubes, proteins or DNA.

Motivations and objectives

The developments above mentioned have resulted in the multiplication of sessions or colloquia

in international meetings. However, workshops on the computational aspects of molecular electronic have been scarce. As emphasized below, a quantitative description of molecular transport needs to integrate several complex effects and it is difficult for a single person/group to gather expertise in all fields. The organization of such a workshop and the discussions between experts in the various aspects of transport have helped in providing a large overview to all participants and in defining the lines of work to be followed. Topics that were discussed include non-exclusively:

Transport formalisms:

Various techniques have been used to calculate transport properties: scattering state formalisms [11-13], equilibrium or non-equilibrium [14-17] Green's function approaches, explicit integration in time of the Schrödinger equation [5,19-21], etc. Comparisons between all these different approaches are scarce in the literature and such a workshop allowed to better understand the connections and differences between available formalisms. Further, in terms of perspective, it was important to discuss the ability of these various techniques to be modified so as to incorporate self-consistency, electron-phonon and electron-electron interactions beyond semi-empirical or standard *ab initio* mean-field approximations. Finally, computer efficiency and the possibility of going towards order-N algorithms [5,18] are important issues discussed for a practical study of realistic systems.

Electron-electron correlations:

From standard Coulomb blockade effects in quantum dots to the Luttinger behavior reported in carbon nanotubes, electron-electron interactions can be crucial in reduced dimensionality systems. Beyond computer-efficient empirical tight-binding, extended Hückel or Hubbard model approaches, state-of-the-art *ab initio* calculations have been so far mainly performed at the DFT level. However, the DFT is a ground state formalism and quantities such as the band gap "offsets" at the contact of two conductors may be severely wrong. Further, the local density approximation is known to misbehave with localized states of the kind encountered in molecular systems. Better descriptions of the exchange-correlation interaction can be included in the Green's function formalisms via the common language of self-energy and attempts to go "beyond DFT" (using for example the GW approximation) have been recently explored [6,22].

Electron-phonons interactions:

In the case of 1D systems, Peierls distorsions and polaronic transport are well known phenomena where electron-phonon coupling is crucial. Electron-phonon coupling may be experimentally studied using STM spectroscopy of adsorbed molecules by taking the second derivative of the current versus appled voltage (Inelastic Electron Tunneling Spectroscopy) [23,24]. But the interpretation of the IETS spectra is matter of a lot of controversies. Further, critical problems to include the electron-phonon coupling are numerous. The complexity of the calculations rapidly increases with the number of vibrational modes involved in the process, and thus with the number of atoms in the molecules. For this reason, and beyond semi-empirical models [8], calculations are presently limited to extremely small molecules (2-3 atoms) [25,26]. Another difficulty is the calculation of the non-equilibrium electronic populations on the molecules and on the leads in presence of inelastic tunneling, in particular taking into account the Pauli principle which must be verified in all the conduction channels. Strategies to include such effects in electronic transport formalisms were discussed.

Some relevant references and recent papers

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Programme

Monday 02

9h-9h30 Welcome

Morning session: Transport formalism
Chair: Kurt Stokbro

9h30-10h15 Hong Guo: Theory and Modeling of Molecular Electronics.
10h15-11:00 George Kirczenow: Understanding molecular wires.
11:00-11:30 Coffee break
11:30-12:15 M. Di Ventra: Transport in Nanoscale Conductors from First-Principles

12:15-14:00 Lunch break

Afternoon session: Transport formalisms continued
Chair: Hong Guo

14:00-14:45 L. Wirtz: Transport through quantum billiards: a model system for ballistic transport in molecules.
14:45-15:30 J. Bernholc: DFT-optimized localized orbitals and nearly O(N) calculations of quantum transport.
15:30-16:15 D. Kosov: Kohn-Sham equations for nanowires with direct current.
16:15-16:45 Coffee break.
16:45-17:30 A. Levy Yeyati: Dynamical Coulomb blockade in nanoscale wires.
17:30-18:15 Jorge Iribas Cerda: Electron transport within the STM context.

Tuesday 03

Chair: J. Bernholc
9:00-9:45 Heiko B. Weber: Experimental aspects of molecular transport

Morning session: DFT calculations.
9:45-10:30 J.J. Palacios: Molecular electronics with Gaussian98: An application to metallic nanocontacts with small molecules.
10:30-11:00 Coffee break
11:00-11:45 F. Evers: How good are DFT-based calculations ?
11:45-12:30 M. Pruneda: Dynamic time-evolution of electrons and nuclei within LCAO

Lunch break

Afternoon session: Electron-phonon interactions and atom relaxations.
Chair: M. Di Ventra

14:00-14:45 Per Hyldgaard: Non-equilibrium Green function calculations of current-induced nanostructure dynamics.
14:45-15:30 H. Ness: Transport in molecular wires with electron-vibration coupling.
15:30-16:15 Tchavdar N. Todorov: Electron-phonon interaction in atomic wires.
16:15-16:45 Coffee break
16:45-17:30 Kristian Thygesen: Stability and transport in monoatomic wires and diatomic contacts

17:30 18:15 N. Lorente: Mode excitation and reaction pathways induced by the STM.

Conference dinner

Wednesday 4

Morning session: Nanotubes and molecular wires
Chair: N. Lorente

9:00-9:45 Klaus Richter: Conductance of single molecule-nanotube hybrids.
9:45-10:30 K. Stokbro: Trans-SIESTA Program
10:30-11:00 Coffee break
11:00-11:45 S. Roche: Electronic transport properties of carbon nanotube based materials and devices.
11:45-12:30 J. Cornil: Negative differential resistance in conjugated molecular wires: a quantum-chemical insight.

Afternoon session: Molecular wires, materials and devices.
Chair: S. Roche

14:00-14:45 A. Ghosh: Silicon-based molecular electronic devices.
14:45-15:30 E. Molinari: Electron states and transport of biomolecular systems for nanodevices
15:30-16:15 J. Taylor
16:15-16:45 Coffee break
16:45-17:30 C. Adessi
17:30-18:15 Risto Nieminen/Martti Puska: Electron transport in layered heterostructures and in 2D nanostructures modeled by Green's functions and finite-element methods.
18:15-19:00 D. Wortmann/S.Bluegel: Spin-dependent ballistic transport from ab-initio Green function embedding.

Thursday 5

Morning session: Electron-electron interactions, dynamical effects
Chair: G. Kircenow

9:00-9:45 Matthias H. Hettler: Current and shot noise in tunneling transport through molecules.
9:45-10:30 X .Blase: Transport through localized orbitals within the GW approximation.
10:30-11:00 Coffee break
11:00-11:45 E.K.U. Gross: Density functional theory of transport properties: static versus time-dependent approach
11:45-12:30 R. Gebauer: A dynamical open-system approach to electron transport.

12h30 Closing session

Coherent transport in molecular wires: how good are DFT based calculations?

F.Evers, F. Weigend, M. Koentopp

Abstract

The experimental value for the zero bias conductance of organic molecules coupled by thio-groups to gold electrodes tends to be much smaller than the theoretical result based on density functional theory (DFT) calculations, often by orders of magnitude. To address this puzzle we consider a special case, namely the organic molecule that has recently been studied experimentally by Reichert *et. al.* (PRL 88, 176804 (2002)) . Our results imply that correlation effects cannot be ignored: a standard step in DFT based transport calculations, namely approximating the electronic ground state wavefunction by a single Slater-determinant with Kohn-Sham-orbitals, is the source for overestimating the width of the experimentally observed conductance peak. However, in the case of HOMO conductance the experimental peak position is still reproduced properly by these calculations provided that nonequilibrium effects on the transmission can be ignored.

A dynamical open-system approach to electron transport

Ralph Gebauer (ICTP Trieste), Roberto Car (Princeton)

Abstract

We present a formulation to electronic transport properties in which a density matrix describing a many-electron system within time-dependent density functional theory is propagated in time under the action of an external electric field. Coupling to a heat bath prevents the system from heating up. The scheme uses periodic boundary conditions which allow us to model a variety of transport geometries. We show applications of this approach to a double-barrier resonant tunneling device. This work has been carried out in collaboration with Roberto Car (Princeton University).

Mode excitation and reaction pathways induced by the scanning tunneling microscope

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Abstract

The scanning tunneling microscope (STM) can induce molecular vibrations. This is detected by changes in the tunneling conductance as the bias voltage matches a vibrational excitation threshold. Vibrational spectroscopy is available for a unique molecule. Nevertheless, the experimental results present several challenges: few modes are detected, certain symmetries are dominant, and site and conformation properties affect the detection. Despite

these difficulties, this technique is proving to be of uttermost importance in the analysis of molecular adsorbates and in their manipulation. We will present a general theory that can predict the outcome of STM induced vibrational spectroscopy. We will analyze the above challenges and show quantitative results. The excitation of localized vibrations can be the precursor of reaction pathways. We will present the first results of mode selected chemistry by tunneling electrons. These results can be understood with the above theoretical treatment enlargened to include vibrational damping and intermode coupling. We will show that intermode coupling is very efficient on metallic surfaces.

Stability and transport in monatomic wires and diatomic contacts

K. S. Thygesen

Abstract

Previous theoretical studies of monatomic C and Na wires, and recent experiments on Au, Pt and Ir wires have shown an even-odd oscillation in the conductance as the number of atoms in the wire is varied. From calculations based on density functional theory (DFT) we infer a similar behavior for Al, although with twice as large a period. The oscillations are explained by a simple model relating the period to the filling of the wire valence band. Recently, Smit et. al. measured a conductance close to $2e^2/h$ of a single hydrogen molecule bridging a pair of Pt electrodes (Nature 419,906). We have studied the stability of such a contact using DFT and find molecular binding energies which for most geometries exceed that of the dissociated molecule. This is interesting since Pt is a widely used catalyst for hydrogen dissociation. We furthermore find that the binding energies decrease as the coordination of the contacting Pt atoms is reduced below 5.

Electron-phonon interaction in atomic wires

Tchavdar Todorov, M. J. Montgomery, J. Hoekstra, A. P. Sutton

Abstract

As part of a long-term project to model current-induced mechanical effects in atomic-scale conductors, we have developed a self-consistent tight-binding model to calculate interatomic forces and electron-phonon scattering rates in current-carrying metallic atomic wires. This model has been applied to two problems. First, we have calculated the inelastic current-voltage spectroscopic characteristics of Au atomic chains (M. J. Montgomery, J. Hoekstra, T. N. Todorov and A. P. Sutton, J. Phys.: Condens. Matter 15 (2003) 731-742). The calculations allow features in the inelastic I-V curves to be related directly to electron interactions with individual phonon modes of the nanojunction. Second, we are setting up dynamical simulations of current-carrying metallic nanojunctions, with current-induced forces and power dissipation included in the simulation. We hope that these simulations will give us insight into current-induced dynamical effects, such as local heating and the influence of current-induced forces on the atomic motion.

Transport through quantum billiards: a model system for ballistic transport in molecules

Ludger Wirtz

Abstract

Wave-function propagation through 2-dimensional billiard-like structures (e.g. in ballistic GaAs/AlGaAs heterostructures [1] or flat microwave cavities [2]) is determined by the geometry of the confining walls and, in particular, by the diffractive coupling to the attached wave-guides. This is similar to the situation of ballistic transport through molecules where the attachment to electrodes induces a coupling between the different transport channels of the unperturbed molecule. In some cases this coupling may have a more pronounced influence on the conductance properties than the composition of the molecule itself. We present a semiclassical model [3] including multiple diffractive scattering between the attached wave-guides for the transmission probability through 2-dim. billiard structures. The theory converges towards the quantum mechanical transmission probability and facilitates an intuitive understanding of the transport properties. [1] C. M. Marcus, A. J. Rimberg, R. M. Westervelt, P. F. Hopkins, and A. C. Gossard, Phys. Rev. Lett. 69, 506 (1992). [2] T. Blomquist, H. Schanze, I. V. Zozoulenko, and H.-J. Stockmann, Phys. Rev. E 66, 026217 (2002). [3] L. Wirtz, C. Stampfer, S. Rotter, and J. Burgdorfer, Phys. Rev. E 67, 016206 (2003).

Silicon-based Molecular Electronic Devices

Avik Ghosh

Abstract

Traditionally molecular electronic efforts, both theoretical and experimental, have focussed on species bonded to gold substrates, exploiting the thiol-gold chemistry. However, recent advances in growing molecules on silicon substrates have opened up the exciting possibility of exploring molecular electronics on silicon. Silicon offers distinctive advantages over its metallic counterparts, because of (a) covalent silicon-carbon bonding-chemistry, (b) absence of metal-induced gap states (MIGS) that considerably improves the electrostatics in molecular devices, and (c) novel physics associated with the band-gap, such as the generation of a new class of resonant-tunneling devices that show negative differential resistance (NDR), with potential circuit applications. Finally, there is the obvious exciting prospect of integrating molecular components into the existing powerful infrastructure of the silicon-based IC industry. In the first part of my talk, I will discuss the general physics of two and three-terminal molecular devices. We have developed an ensemble of computational simulation tools, from simple semi-empirical theories to rigorous "first-principles" DFT calculations based on coupling nonequilibrium Green's function (NEGF) transport formalisms self-consistently to available quantum chemical codes. While the former gives us quick and simple results that capture the essential physics of nanotransport and offers qualitative insights, the latter generates I-V characteristics with no adjustable parameters. We will see that the essence of these I-Vs can be described in terms of simple parameters such as the contact Fermi energy, the molecular levels and their broadenings, the capacitive couplings

with the contacts and the charging energy. I will apply these concepts to analyze the electrostatic and conformational gating of a molecular transistor. Ultrashort molecular transistors suffer from poor electrostatics due to the gate oxide thickness and MIGS from the contacts. Utilizing conformational degrees of freedom offers clear advantages, increasing the transconductance and eliminating competition among the electrodes through the vector directionality of the molecular dipoles. However, room temperature conformational transistors suffer from thermal fluctuations, generating a fundamental limit on conformational transistor efficiency within traditional CMOS design principles. In the last part of my talk, I will describe the physics of molecular components grown on silicon, specifically, a novel molecular RTD, for which preliminary experimental evidence has been reported by Mark Hersam's group at Northwestern University. A common problem encountered in simulating contact-molecule heterostructures is that the atomic basis sets that do justice to the chemistry of a molecule is quite a poor choice for describing the bandstructure of bulk contacts; on the other hand, injudiciously invoking two different basis sets for the two parts is likely to create interfacial problems. I will discuss a formalism that we have developed to handle the mixed basis-set problem in a seamless way. Based on this formalism, we provide a first-principles calculation of the STM current through a molecule (styrene and TEMPO) grown on Si(100) surfaces. I will show that the presence of the silicon band-edge gives a molecular RTD with prominent NDR peaks that arise from the molecular levels. Furthermore self-consistent charging could create hysteresis in the NDR peak positions.

Transport in Nanoscale Conductors from First Principles

Massimiliano Di Ventra
Department of Physics, Virginia Tech

Abstract

Electronic transport is a challenging problem when one wants to solve it from first principles. Physical issues that need to be considered include coherence effects, current fluctuations, local heating, current-induced forces, and so on. To complicate matters electric current does not generally satisfy a minimum principle [1]. I will present a theoretical approach that addresses the above issues. The approach is based on the self-consistent solution of the Lippmann-Schwinger equation [2] within the density functional theory of many-electron systems for a sample connected to metallic electrodes with a finite bias. The formalism provides the most fundamental quantities to describe the dynamics of the whole system: the self-consistent electronic wave functions. From these wave functions, all physical quantities of interest can be derived. To exemplify the approach I will present results on coherence effects [3], current-induced forces [4], coupling to low-energy bosons [5], shot noise, [6] and local heating [7] in selected atomic and molecular wires. Work supported in part by NSF, Carilion Biomedical Institute and ACS-Petroleum Research Fund. [1] Z. Yang, A. Tackett, M. Di Ventra, Phys. Rev. B 66, 041405 (2002). [2] N.D. Lang, Phys. Rev. B 52, 5335 (1995); M. Di Ventra and N.D. Lang, Phys. Rev. B 65, 045402 (2002). [3] M. Di Ventra, S.T. Pantelides, and N.D. Lang, Phys. Rev. Lett. 84, 979 (2000); M. Di Ventra, S.T. Pantelides, and N.D. Lang, Appl. Phys. Lett. 76, 3448 (2000) [4] M. Di Ventra and S.T. Pantelides, Phys. Rev. B 61, 16207 (2000); M. Di Ventra, S.T. Pantelides, and N.D. Lang, Phys. Rev. Lett. 88, 046801 (2002); Z. Yang and M. Di Ventra, submitted. [5] M. Di Ventra, S.G. Kim, S.T. Pantelides, and N.D. Lang, Phys. Rev. Lett. 86, 288 (2001). [6] Y.-C. Chang and M. Di Ventra, submitted. [7] Y.-C. Chang, M. Zwolak, M. Di Ventra, submitted.

3.2.2 Report on MgB_2 Workshop in Rome

Open questions in understanding the superconducting and normal-state properties of MgB_2

Università degli Studi di Roma 'La Sapienza'
Dipartimento di Fisica

Rome 2 – 4 July 2003

Supported by ESF Psi-k Programme

The research on MgB_2 has been an international effort from the beginning, which is also reflected in the large number of countries (12) from which the participants of the workshop came. The distribution of participants based on their home institution shows that most of the participants came, as expected, from Italy (19), followed by the USA (7), France (5), Switzerland (5), Germany (4), UK (3), and Mexico (2). From the following countries only one person participated: Czech Republic, The Netherlands, Japan, Israel and Russia. In order to create an atmosphere fruitful for discussion the number of participants had been limited to 50 persons.

The main goal of the workshop has been to bring together the experts working in the field of MgB_2 in order to define the current status of our understanding of this material and to discuss future directions for research. In order to achieve a high quality and well balanced selection of the ongoing research worldwide the majority of the 28 oral presentations were given in form of 22 invited talks of 30 min each, and the remaining 6 shorter talks have been selected from the submitted abstracts. Further, there were 8 poster presentations. The 22 invited speakers came from institutions based in Germany, Italy, France, Japan, The Netherlands, Switzerland, Great Britain and USA. A large number of interesting experimental and theoretical findings were reported, many of them indicating problems in the current understanding. The titles and abstracts of all invited and contributed talks and posters are given in the book of abstracts. Therefore we will not give a detailed discussion of each talk in the following but only mention the most important problems and discussions not covered by the book of abstracts.

The first day was devoted to the electronic structure and phonons in MgB_2 and related compounds. The talks on the theoretical calculation and experimental determination of the Fermi surface in MgB_2 gave a nice example of the interplay between experiment and theory, and of its importance for our understanding. At the same time it also clearly indicated the limits of the accuracy of our computational tools. Drechsler raised an interesting issue of a shift of the electronic bands due to polaronic effects which are neglected in current density-functional theory implementations. A different shift of the σ-bands in respect to the π-bands in MgB_2 could resolve the small discrepancies between experiment and theory which still exist. The results on the anharmonicity of the important boron-boron optical bond stretching E_{2g} mode in MgB_2 reported by Mauri indicated another problem in our current models. According to these calcu-

lations the total anharmonic enhancement of this phonon mode is only about 5% and not 15% as generally believed. This poses problems for the explanation of the isotope effect which relies on the larger value of the anharmonic enhancement.

The main evening highlight has been the 75 min open discussion which turned out extremely lively, and was only limited by the closing of the conference building at 19:00. The first evening focused on the following question: *Are there other materials beside MgB_2 which would show similar superconducting properties?* A theoretically suggested material, hole-doped LiBC, has been discussed. There are several groups worldwide which were able to produce LiBC, although there are no reports of successful hole doping by partially removing Li atoms without structural changes. One problem seems to be clustering of the Li vacancies which leaves large parts of the crystal undoped but changes locally the properties in an uncontrolled way. Theoretical input on the dynamical crystal stability as function of realistic vacancy concentrations may be helpful for further progress. Connected with this more materials-science oriented problem is the problem of impurity doping in MgB_2 as enthusiastic reminded by Canfield. Surprisingly, there are only two successful dopants (Al and C) in MgB_2, although there have been many attempts with practically all other elements of the periodic table. Canfield not only indicated the problem but proposed a possible route, by crystal growth from a solution, to introduce more dopants in MgB_2. This would be very important for future progress in the field, because theory expects a strong effect of impurities on the superconducting and normal-state properties. Research in this area seems to be very promising and will hopefully be supported by funding agencies in the future.

The presentations on the second and third day were directed to various topics with the main emphasis on impurity effects and the influence of magnetic field. Again, most of the talks presented exciting findings stimulating the evening discussion.

The influence of impurities on the physical properties of MgB_2 have been a hot topic in the presentations and discussions. The results obtained from specific heat measurements and tunneling (also several reports during the last day) on the two-gap behavior in MgB_2 reported by different groups showed a remarkable qualitative and even quantitative agreement. While the larger gap follows the theoretical predictions, the smaller one is practically sample-independent. This is in sharp contrast to the widely accepted two-gap model, which predicts the merging of the superconducting gaps due to impurity scattering. So far there is no theoretical explanation of the observed behavior. On the other hand the results reported by Putti showed a direct confirmation of the theoretical predicted disorder effects on the temperature dependence of the resistivity in the two-band model. The observed change in the slope of the resistivity after irradiating samples can be understood as the change from a relatively clean sample before irradiation in which the π-bands contribute most to the conductivity. The irradiation creates many defects which affect the π-band more and make the conductivity in that band very small. Therefore the conductivity is now determined by the σ-band which exhibits a different temperature dependence than the π-band, resulting in a change of the temperature dependence of the resistivity. The theoretical work by Golubov indicated changes in the superconducting density of states due to impurity scattering. This could have profound consequences on the analysis of experimental results from specific-heat measurements. The standard assumption of two BCS-

like densities of states used in practically all fits of the specific heat data breaks down. This also represents a possible starting point for an explanation of the unexpected behavior of the two gaps, mentioned above. Further work in that direction is required in order to elucidate the qualitative and quantitative implications of that finding. Therefore also from the theoretical point of view it is very worthwhile to study the influence of impurities.

The evening discussion centered also around the above-mentioned problems in detail. There were further discussions on the importance of non-adiabatic effects which are currently not included in the standard theory of superconductivity of that material. In the following we list the main topics of the discussions which were regarded most important by the participants.

1. Are there other materials, besides MgB_2, which would show similar superconducting properties?

2. The small gap as function of T_c is roughly a constant. Moreover, this seems to hold for irradiated samples and C- or Al-doped samples.

3. According to recent first-principles calculations and inelastic X-ray scattering measurements the anharmonic enhancement of the E_{2g} is only 5%. In that case the reduced isotope effect becomes a mystery. Two-phonon processes and non-adiabatic effects may play a role here.

4. There are still some discrepancies between theoretical calculations and the de-Haas-van-Alphen measurements. While most of the observed orbits are explained very well, there is one orbit (F3) whose angular dependence shows unaccounted deviations from th theoretical calculations. Further, the Stoner enhancements in different bands, observed experimentally, varies much stronger than the calculated enhancement.

5. The tunneling experiments agree among themselves on $\Delta_\pi = 2.7 \pm 0.2$ meV, and Andreev reflection measurements on 2.1 ± 0.2 meV, roughly. Why is there such a difference between the two methods?

6. What are the limiting effects of the Born-Oppenheimer approximation on the electronic structure calculations? What is the influence of nonadiabatic effects?

This meeting has been very important for the MgB_2 research community. Practically all leading groups working experimentally or theoretically in the field have been brought together. For the first time it was possible to show that the latest results from the different groups now start to converge to the same quantitative results. This is true not only, for example, for the measurements of the superconducting gaps and other properties, but also for theoretical calculations. The importance of this convergence of results should not be underestimated. Now we have reliable numbers from experiment against which the accuracy of the theoretical understanding can be tested. While there is good qualitative and sometimes even quantitative agreement between theory and experiment, there are still some gaps in our understanding. Currently it is not clear if the observed discrepancies can be resolved by minor improvements of the current theoretical framework, or if they are the first sign of interesting physics missed so far. Certainly, more work is required to answer this question. If one has to pick a single most

important topic, the doping behavior and influence of impurities has been the hottest topic from the experimental, as well as from the theoretical point of view. This can be seen as a general consensus of the workshop participants for future research directions in the field of multiband superconductivity.

While there are no answers yet available for the above-raised questions, it was very important to define the current status of what we know from experiment and theory. This goal has been achieved and makes the workshop already a successful one. Even more, there were several new ideas discussed how to make further progress in experiment and theory, which will certainly be tried out in the near future. From the personal feedback from many participants we believe that the workshop has been very fertilizing for the field.

We would like to thank the European Science Foundation and the **ESF Psi-k program**, the INFM Center for Statistical Mechanics and Complexity, and the Department of Physics of the University of Rome "La Sapienza", which made this exciting workshop possible.

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Conference Program

02 July 2003

8:30-9:00 *Registration*

9:00-9:15 **G. Parisi / G. B. Bachelet / L. Pietronero**
Welcome greeting and opening remarks

Chairman: **L. Pietronero**

9:15- 9:50 **O. K. Andersen** (Stuttgart, Germany)
What is special about the electronic structure of MgB_2?

9:50-10:30 **I. I. Mazin** (Washington DC, USA)
An overview of the theory of superconductivity in MgB_2

10:30-11:00 * Coffee break *

Chairman: **S. Savrasov**

11:00-11:35 **A. Carrington** (Bristol, UK)
De Haas-van Alphen determination of the Fermi surface parameters of MgB_2

11:35-12:10 **S. L. Drechsler** (Dresden, Germany)
Aspects of LDA electronic structure, electron-phonon related properties and superconductivity in AB_2 (A= Mg, Zr, Ta)

12:10-13:40 * Lunch break *

Chairman: **P. Canfield**

13:40-14:15 **W. Pickett** (Davis, USA)
Alloying, Strain, and Extreme Electron-Phonon Coupling in the MgB_2 Class of Superconductors

14:15-14:50 **S. Massidda** (Cagliari, Italy)
Phonon and electron-phonon renormalization in Al doped MgB_2

14:50-15:25 **E. Cappelluti** (Rome, Italy)
Small Fermi energy, anharmonicity and nonadiabaticity in MgB_2 and related compounds

15:25-15:55 * Coffee break *

Chairman: **W. E. Pickett**

16:00-16:35 **M. D'Astuto** (Grenoble, France)
Phonon dispersion and lifetimes in MgB_2 and $Mg_{1-x}Al_xB_2$

16:35-17:10 **P. Postorino** (Rome, Italy)
Raman investigation of $Mg_{(1-x)}Al_xB_2$:
effects of Al content and pressure on the phonon spectra

17:10-17:30 **F. Mauri** (Paris, France)
Role of anharmonicity in phonon frequencies
and lifetimes of MgB_2

17:30-18:45 Discussion

03 July 2003

Chairman: **J. Kortus**

9:00-9:35 **K. P. Bohnen** (Karlsruhe,Germany)
Lattice dynamics and Electron-Phonon Coupling in Diborides

9:35-10:10 **A. A. Golubov** (Twente,The Netherlands)
Two-band Eliashberg model for MgB_2

10:10-10:40 * Coffee break *

Chairman: **A. D. Caplin**

10:40-11:15 **P. Canfield** (Ames, USA)
Thermodynamic and transport properties of pure
and substituted MgB_2

11:15-11:50 **A. Junod** (Geneva, Switzerland)
Multiple gaps in MgB_2 and elsewhere:
the information given by measurements of the specific heat
versus magnetic field, orientation and disorder

11:50-12:25 **A. V. Sologubenko** (Zurich,Switzerland)
Thermal conductivity of MgB_2 and multigap superconductivity

12:25-14:00 **Posters and Lunch break**

Chairman: **A. Junod**

14:00-14:35 **T. Masui** (Tokyo, Japan)
The electronic properties of C-subsituted MgB_2 single crystals

14:35-14:55 **E. Pavarini** (Pavia, Italy)
Theory of normal state NMR in $Mg_{1-x}Al_xB_2$

14:55-15:10 **H. Schmidt** (Argonne, USA)
Disorder Effects in MgB_2 Using SIS Tunneling Spectroscopy

15:10-15:25 **M. Putti** (Genova, Italy)
The effect of disorder and doping on gap amplitudes
and relaxation rates of σ and π bands

15:25-16:00 * Coffee break *

Chairman: **I. I. Mazin**

16:00-16:35 **A. D. Caplin** (London, UK)
Critical fields of MgB_2

16:35-16:50 **A. Gurevich** (Wisconsin, USA)
Enhancement of the upper critical field in the two-gap superconductor MgB_2 by selective tuning of impurity scattering

16:50-17:25 **M. R. Eskildsen** (Geneva,Switzerland)
Vortex studies in Magnesium Diboride: Effects of Doping and Anisotropy

17:25-17:40 **A. Bianconi** (Rome, Italy)
T_c amplification at the shape resonance in doped MgB_2

17:40-18:45 Discussion

04 July 2003

Chairman: **A. A. Golubov**

9:00- 9:35 **R. S. Gonnelli** (Torino, Italy)
Directional point-contact spectroscopy in MgB_2 and $Mg_{1-x}Al_xB_2$ single crystals: comparison to the predictions of the two-band model

9:35-10:10 **A. G. M. Jansen** (Grenoble, France)
Andreev-reflection study in MgB_2

10:10-10:25 **S. Kuzmichev** (Moscow, Russia)
Experimental evidence of two-band behavior of MgB_2

10:25-11:00 * Coffee break *

Chairman: **R. S. Gonnelli**

11:00-11:35 **M. Iavarone** (Argonne, USA)
STM Tunneling spectroscopy in MgB_2

11:35-12:10 **S. Savrasov** (Newark, USA)
Superconductivity in MgB_2 and $MgCNi_3$: two opposite cases

12:15-12:30 O. K. Andersen: Concluding remarks

12:30-14:00 * Lunch break *

What is special about the electronic structure of MgB_2?

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Abstract

In contrast to other sp^2-bonded materials, MgB_2 has holes at the top of the boron bonding σ-bands. This is due to lowering of the π-bands by the Mg^{++} ions. The σ-holes are in two narrow, zone-centered Fermi cylinders and couple strongly to the phonons with $q_\parallel < 2k_F$ in the two optical boron-boron bond-stretching branches, the E_{2g}-phonons. This interaction between a few holes and a few phonons is the dominant electron-phonon interaction in MgB_2 and its coupling constant is: $\lambda_{\sigma\sigma} = N_\sigma D_\sigma^2/M\omega^2$. This expression, first employed by Pickett, is useful for understanding the materials trends, and we shall show that it is also very accurate. N_σ is the density of states of the σ-holes at the Fermi level, ω is the energy of the E_{2g}-phonons, D_σ is their deformation potential splitting the σ-bands at $k_\parallel = 0$, and M is the reduced mass. $\lambda_{\sigma\sigma}$ not only gives the electron-phonon scattering which dominates the Eliashberg functions and the σ-contribution to the mass enhancement of the σ-holes, but also the σ-contribution to the softening of the E_{2g}-phonons. Since $\lambda_{\sigma\sigma} + \lambda_{\pi\pi} \sim 0.7 + 0.3 = 1$, ω^2 is reduced by a factor ~ 3, and that is the reason –next to D_σ being large– why $\lambda_{\sigma\sigma}$ is relatively large. The σ-contribution to the softening is caused by the transfer of holes between the two σ-bands upon adiabatic E_{2g}-displacement. This transfer stops when the splitting at $k_\parallel = 0$ exceeds the Fermi energy and, as pointed out by Boeri et al, that causes anharmonicity and a reduction of the softening when the number of σ-holes is so small that $\varepsilon_F \lesssim tD_\sigma$. Here, $t \equiv \sqrt{\hbar/M\omega}$ is the turning point of the E_{2g} zero-point motion. As a result, $\omega^2 \approx \omega_0^2 \left(1 + 2\lambda_{\sigma\sigma}\frac{N_\sigma+N_\pi}{N_\sigma+2N_\pi}\left[1 - \mathrm{erf}\left(\frac{\varepsilon_F}{tD_\sigma}\right)\right]\right)/(1 + 2\lambda_{\sigma\sigma} + 2\lambda_{\pi\pi})$, where ε_F is the average between the σ-band energies at Γ and A. In MgB_2, this anharmonicity effect reduces $\lambda_{\sigma\sigma}$ from 0.96 to 0.72. That might be undone by additional hole doping. The same effect is the likely cause for the observed decrease of T_c with decreasing number of holes, since N_σ is fairly independent of energy (when $\varepsilon < \varepsilon_\Gamma$) because the σ-bands are nearly parabolic in two-dimensions and nearly constant in the third. Another peculiarity of MgB_2 is that upon decreasing the number of holes, the number of E_{2g}-phonons decreases as $(2k_F)^2$, but their widths increase as $\lambda_{\sigma\sigma b}\,(2k_F)^{-2}$. The contributions to the electron-phonon interaction from all other phonons and from interactions involving the π-electrons, are all together smaller than $\lambda_{\sigma\sigma}$. The second thing special about the electronic structure of MgB_2 is that for common impurities, the rate for scattering between the σ and π-bands is orders of magnitude smaller than the intraband scattering rates. As a result, MgB_2 has two gaps which close at a common $T_c \approx 40$ K due to phonon-mediated interband scattering. The Eliashberg equations allowing for two order parameters, together with energy bands, electron-phonon interactions, and the matrix-structure of the retarded Coulomb pseudopotential all calculated from density-functional theory, explain nearly all physical properties observed sofar for MgB_2 and similar materials. The basic reasons for the negligible $\sigma\pi$ impurity scattering are the disparity of the σ and π Wannier functions and the fact that the holes are close to the top of the σ-bands, as we shall explain and also illustrate with calculations.

T_c amplification at the shape resonance in doped MgB_2

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Abstract

The $A_xMg_{1-x}B_2$ system (A=Al,...) has been studied by high-resolution x-ray diffraction measurements to explore the superconducting phases of the high T_c diborides as a function of the number of holes in the sigma band and B-B microstrain. The superconducting transition temperature varies from 3.5 K in $AlMgB_4$ to 39.5 K in MgB_2. The model of two channel superconductivity has been applied to the $Al_{1-x}Mg_xB_2$. The evolution of interband coupling parameter as a function of x shows a maximum at the 'shape resonance', where the Fermi surface changes from 2D to 3D topology. While in MgB_2 the quantum interference effects give an amplification of T_c by a factor of 2 in comparison with the dominant intraband single channel pairing, in $AlMgB_4$ the interband coupling gives an amplification of about 100 times. The experimental variation of the ratio between the two gaps as a function of x is a good test for the key role of the interband pairing near the band edge.

Lattice dynamics and electron-phonon coupling in diborides

K.P. Bohnen, R. Heid and B. Renker
Forschungszentrum Karlsruhe, Institut für Festkörperphysik

Abstract

A brief review of the lattice dynamics and electron-phonon coupling in diborides is presented based on ab-initio density-functional calculations. We show results for phonon dispersions and electron-phonon spectral functions and discuss their implications for superconducting properties in the isotropic limit. Results are presented for MgB_2, AlB_2 and $MgAlB_4$ as well as for a wide class of transition metal diborides. Although comparison with experimental data usually indicates very good agreement concerning the lattice dynamics this is not always the case for the calculated T_c values indicating the necessity of further studies.

The anisotropy and magnetic field dependence of the two gaps in MgB_2

Y. Bugoslavsky, Y. Miyoshi, G.K. Perkins, L.F. Cohen, A.D. Caplin
Imperial College London

Abstract

The interplay between two superconducting gaps in MgB_2 in applied magnetic field is an issue that can provide further insight into the microscopic properties of this material. There has been experimental evidence (from point-contact spectroscopy and heat capacity) which has been interpreted as an indication of an abnormally small additional critical magnetic field, at which superconductivity in the π band is suppressed. This effect would have strong implications, for example, on the structure of magnetic vortices, hence on magnetic properties in the mixed state. However no trace of a change in magnetic behaviour at this "π-band H_{c2}" has been reported. In this work we address the question of the field-dependence of the σ- and π-band gaps and their anisotropy. We have performed point-contact measurements on high-quality MgB_2 films grown by hybrid physical chemical vapour deposition at PennState University. The films were on Al_2O_3 substrates, had T_c of 39K and the resistivity at 40 K was around 10 mOhm cm. The films were well textured, so it was possible to measure the anisotropy of H_{c2}, which was approximately equal to 4 at T close to T_c, with a slow increase at lower temperatures. The point contacts were created by pressing a sharp gold tip to the film surface. Magnetic field up to 8 T was applied either parallel or perpendicular to the film. Although the injection of electrons from the tip was nominally parallel to the c-axis of the film, where (according to the theory) only the π-band gap should be involved, we clearly saw well-resolved two-gap spectra, indicating that the actual injection was in a rather wide cone, and that there was efficient coupling to the σ-band gap as well. At 4.2 K and at fields up to 3 T the spectra were extremely well-defined, so that they could be fitted to the BTK model very robustly. We can definitely conclude that the π-band gap does not close at a small field; indeed there is only little variation of the value of this gap up to 3 T. However the amplitude of the associated spectral peaks certainly gets suppressed in field, which is a result of increasing effective smearing. This can be attributed to an additional field-induced pair-breaking mechanism, which is most likely due to single-particle excitations in the vortex cores. The retention of the π-band gap was observed for both field directions. We discuss how these results can be reconciled with the heat capacity measurements.
This work is supported by the UK Engineering and Physical Sciences Research Council.

Thermodynamic and transport properties of pure and substituted MgB_2

P. Canfield

Ames Laboratory and Departement of Physics, Iowa State University

Abstract

I will review some of the basic thermodynamic and transport properties of high purity, polycrystalline samples of MgB_2, ranging from normal state transport to the anisotropy of the upper critical field. I will then present the results of recent work on the effects of chemical substitutions, in particular the effects of carbon substitution for boron. Whereas great care has to be taken to insure that the boron and carbon are mixed at an atomic level, once this has been accomplished a clear and reproducible suppression of T_c from $\sim 40K$ for pure MgB_2 to $\sim 22K$ for $Mg(B_{0.9}C_{0.1})_2$ can be achieved. Despite this strong suppression of the superconducting state there is clear evidence for the continued existence of the two gap, superconducting ground state that is found in pure MgB_2.

Critical fields of MgB_2

A.D. Caplin
Imperial College London, UK

Abstract

It is now well-established that the upper critical field H_{c2} of nominally-pure MgB_2 rather low, and that the anisotropy between the ab-plane and the c-direction is modest. An alternative description of a "nominally-pure" sample is that the impurity species and concentration are essentially unknown; consequently it is not too surprising that the reported $H_{c2}(T)$'s do show some variation. The lower critical field H_{c1} is rather more difficult to measure, but does show clearly that the Ginzburg-Landau k is quite small, so that clean MgB_2 is only just a Type II superconductor. Simple-minded estimates of the electron mean free path l and the coherence length x indicate that these "pure" samples are well into the clean limit, and so suggest that there is considerable scope for enhancement of H_{c2} - as is vital for utilisation of MgB_2 in conductor applications - through the introduction of strong electron scattering. This scenario is complicated greatly, and apparently beneficially, by the double-gap nature of the superconducting state in MgB_2, and the large difference between inter- and intra-band scattering rates. Recent experiments on the impact of additional scattering on the critical fields of MgB_2 will be reviewed, and compared with the impact of scattering on the microscopic gaps.
This work has been supported by UK Engineering and Physical Sciences Research Council. I am indebted to my colleagues Dr Yura Bugoslavsky, Dr Lesley Cohen, Mr James Moore and Dr Garry Perkins for their experimental data and for extensive discussions.

Small Fermi energy, anharmonicity and nonadiabaticity in MgB_2 and related compounds

E. Cappelluti, L. Boeri, G.B. Bachelet, C. Grimaldi and L. Pietronero
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Abstract

Superconductivity at $T_c \simeq 40$ K in MgB_2 is thought to origin from the strong electron-phonon coupling of the σ-bands, whereas the residual interband scattering gives rise to the multigap phenomenology. The extremely low charge density of the σ-bands is reflected in the small Fermi energy E_F^σ, a fraction of eV, a common feature which is shared also by cuprates and fullerides. In the present contribution we analyze the anomalous effects arising from the small Fermi energy phenomenology, when E_F^σ becomes comparable with the other energy scales of the systems. In particular we show that the anharmonic character of the E_{2g} phonon mode is strictly related to the smallness of the Fermi energy with respect to the electron-phonon coupling $g_{E_2 g}$: $E_F^\sigma \sim g_{E_2 g}$. We discuss also the nonadiabatic effects arising from the finite adiabatic ratio $\omega_{\rm ph}/E_F^\sigma$ as well as nonadiabatic effects induced by zero point quantum fluctuations.

De Haas-van Alphen determination of the Fermi surface parameters of MgB_2

A. Carrington
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Abstract

In this talk I will review our measurements of de Haas-van Alphen (dHvA) oscillations in single crystals of MgB_2. The analysis of these oscillations provides a precise check of band-structure calculations, as well as a measure of the many body electron-phonon interactions, which enhance the quasi-particle effective masses and give rise to superconductivity. Six of the nine possible orbits were observed on all four sheet of Fermi surface. We are therefore able to show that to a good accuracy the calculated Fermi surface of MgB_2 is correct. The differences with calculation are small (in terms of $\Delta k_f/a^*$) but show that the σ hole pockets hold some 16% less holes than calculations would suggest. By comparing the measured quasi-particle effective masses with the calculated band masses we find that the electron-phonon coupling strength λ is a factor ~ 3 larger on *both* the 2D σ orbits than on *both* the 3D π orbits, in accord with calculations. Finally, we discuss data for the damping of the dHvA signal on the π tubes by the opening of a superconducting gap near H_{c2}.

Band-filling effects on electron-phonon properties of normal and superconducting state

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Abstract

We address the effect of band filling on the effective electron mass m^* and the superconducting critical temperature T_c in a electron-phonon system. We compare the vertex

corrected theory with the non-crossing approximation of the Holstein model within a local approximation. We identify two regions of the electron density where m^* and T_c are enhanced or decreased by the inclusion of the vertex diagrams. We show that the crossover between the enhancement at low density and the decrease towards half filling is almost independent of the microscopic electron-phonon parameters. These different behaviors are explained in terms of the net sign of the vertex diagrams which is positive at low densities and negative close to half filling. Predictions of the present theory for Al doped MgB_2, which is argued to be in the low density regime, are discussed.

Phonon dispersion and lifetimes in MgB_2 and $Mg_{1-x}Al_xB_2$

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Abstract

We present measurement of phonon dispersion and linewidth in a single crystal of MgB_2 along the Γ-A, Γ-M and A-L directions using inelastic X-Ray scattering (IXS) [A. Shukla *et al. Phys. Rev. Lett.* **90**, 095506 (2003)]. The effect of both electron-phonon coupling and anharmonicity on the linewidth are calculated using Density Functional Theory, obtaining excellent agreement with experiment. The dominant contribution to the linewidth is always the electron-phonon coupling. We also present recent results of phonon dispersion and linewidth on single crystals of $Mg_{1-x}Al_xB_2$ by IXS [H. Schober *et al.* unpublished results]. In this study, we observe the evolution of the energy and the broadening of the optical modes upon Al doping, from the low content superconducting phase ($x < 0.5$) to the high content non-superconducting phase ($x > 0.5$).

Effect of Aluminum and Carbon doping on the structural and electronic properties of superconducting MgB_2

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Abstract

Experiments have shown that the superconducting critical temperature of MgB_2 decreases for both Al and C substitutions. In both cases we have electron doping since Al and C have one electron more than Mg and B, respectively. The mechanism explaining the reduction of T_c in electron doped-MgB_2 currently is in debate. In this work, we have studied the structural and electronic properties of $Mg_{1-x}Al_xB_2$ and $MgB_{2-x}C_x$ using the ab-initio Virtual Crystal Approximation. The results were obtained by means of first-principles full-potential total-energy calculations. Results for the lattice parameters and the electronic structure as a function of the electron doping, are presented. The Fermi surface associated with holes

at the boron planes, gradually collapses with Al and C doping and dissappears for the critical concentrations of x(Al)=0.56 and x(C)=0.35, respectively. More interestingly, we find that in both Al and C doped MgB_2, the experimental data for the superconducting critical temperature scale with the calculated Fermi surface area of the σ-band. This result indicates that the experimentally observed loss of superconductivity in $Mg_{1-x}Al_xB_2$ and $MgB_{2-x}C_x$ is a direct consequence of the σ-band filling.
This research was supported by Consejo Nacional de Ciencia y Tecnologia (CONACYT, Mexico) under Grant. No. 34501-E.

Ab-initio evidence of intrinsic anharmonicity in superconducting Al-doped MgB_2

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Abstract

Al-doped MgB_2 forms a solid solution with MgB_2 and AlB_2 at the ends, thus $Mg_{1-x}Al_xB_2$ is a key system for understanding the origin of the anomalous properties and superconductivity in MgB_2. Recent calculations based on the ab-initio Virtual Crystal Approximation shown that $T_c(x)$ scale with the σ-band Fermi surface area, and that the collapse of the FS at x=0.56 correspond to the critical concentration where the superconducting phase disappears. In the present work we have studied the dynamic of the E_{2g} phonon mode as a function of Al doping using the Frozen Phonon Approximation. The results were obtained by means of first-principles full-potential total-energy calculations. We find that starting from AlB_2, a sharp harmonic-anharmonic transition occurs at the critical concentration x=0.56, which correlates with the onset of superconductivity in $Mg_{1-x}Al_xB_2$. In addition, we find that this harmonic-anharmonic transition is accompanied of a strong phonon frequency renormalization. The results show that the anharmonicity of the E_{2g} phonon mode is intrinsic to the superconducting phase in $Mg_{1-x}Al_xB_2$. Indicating that the position of the σ-band with respect to the Fermi level is the key parameter controling the electronic, phononic, and superconducting properties in Al-doped MgB_2.
This research was supported by Consejo Nacional de Ciencia y Tecnologia (CONACYT, Mexico) under Grant. No. 34501-E.

Aspects of LDA electronic structure, electron-phonon related properties and superconductivity in AB_2 (A= Mg, Zr, Ta)

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Abstract

Within the local density approximation (LDA) we report full potential calculations of the Fermi surfaces areas and band masses of MgB_2 and ZrB_2. Some discrepancies in areas in MgB_2 with respect to dHvA data [1] can be removed by a small shift of s-bands relative to p bands. It is ascribed to the much stronger electron-phonon inter-action (EPI) in the former subsystem. Comparison of effective masses lead to orbit averaged EPI coupling constants λ= 0.84 to 1.19 on the σ-tubes and λ=0.26 to 0.37 on π-derived Fermi surface sheets (FSS), whereas for ZrB_2 only weak EPI coupling $\lambda < 0.2$ is found. Similar values of the EPI coupling constants were found theoretically using the deformation potential method and other techniques. The ARPES data of MgB_2 [2,3] can be also well described by the LDA showing the presence of surface states. A proximity model for the interplay of bulk and surface superconductivity is proposed. The role of a sizable Fermi velocity anisotropy on certain FSS for the upper critical field anisotropy $H_{c2}(T)$ is discussed in terms of multiband superconductivity. In the bulk MgB_2 case the v_F-anisotropy of the strongly interacting holes on the σ-tubes dominates the temperature dependent H_{c2} anisotropy which is somewhat reduced by the coupling to the nearly isotropic π derived Fermi surface sheets. A comparison with other available experimental data such as critical fields, specific heat, transport, optical, point-contact and tunneling is made. No bulk superconductivity is found for ZrB_2 and TaB_2. The possibility of surface superconductivity in these systems is discussed

[1] A. Carrington *et al.*, cond-mat-0304435

[2] H. Uchiyama *et al.*, Phys. Rev. Lett. 88 157002 (2002)

[3]S. Suoma *et al.*, Nature 423, 65 (2003)

Vortex studies in Magnesium Diboride: effects of doping and anisotropy

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Abstract

Recent results of vortex studies in MgB_2 are presented. Scanning tunneling spectroscopy (STS) was used to image the vortices in aluminum-doped MgB_2, with the tunnel current and applied field parallel to the c axis. This tunneling direction couples essentially only to the π band. Doping with 2-3% Al leads to a reduction of T_c as well as H_{c2}. We find that the superconducting gap in the π band is increased compared to pure MgB_2. Consistent with this the coherence length, determined from the vortex size, is found to decrease. STS vortex imaging in pure MgB_2, with the tunneling current and field perpendicular to the c axis, revealed a distorted hexagonal vortex-lattice. The distortion is determined by the penetration depth anisotropy, which is found to be much smaller than the upper critical field anisotropy. Finally, small-angle neutron scattering (SANS) was used to study the vortex-lattice over a wider field and temperature range. For $H \,||\, c$ a 30° vortex-lattice reorientation transition was discovered, coinciding with a suppression of superconductivity in the π band. Applying the field at 45° away from the c axis, showed a vortex-lattice anisotropy which increases as a function of field as well as temperature. All the effects outlined above will be discussed in the talk, and shown to be clear effects of two-band superconductivity.

Effect of two bands on critical fields in MgB_2 thin films with various resistivity values

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Abstract

Upper critical fields of four MgB_2 thin films were measured up to 28 Tesla at Grenoble High Magnetic Field Laboratory. The films were grown by Pulsed Laser Deposition and showed critical temperatures ranging between 29.5 and 38.8 K and resistivities at 40 K varying from 5 to 50 mWcm. The critical fields in the perpendicular direction turned out to be in the 13-24 T range while they were estimated to be in 42-57 T the range in ab-planes. In contrast to the prediction of the BCS theory, we did not observe any saturation at low temperatures: a linear temperature dependence is exhibited even at lowest temperatures at which we made the measurements. Moreover, the critical field values seemed not to depend on the normal state resistivity value. In this work, we analyze these data considering the multiband nature of superconductivity in MgB_2 We will show how the scattering mechanisms

that determine critical fields and resistivity can be different. This explains why films with resitivities differing by one order of magnitude can show similar critical fields.

Simplest tight binding for $Al_xMg_{1-x}B_2$ in-plane phonons

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Abstract

The simplest tight-binding model of a graphene sheet allows us to understand the dependence of the phonon frequencies and of anharmonicity in MgB_2 and similar compounds on the filling of the σ bands and on the exchanged phonon wave-vector. Leaving the electronic bands and the repulsive term of the total energy unchanged, we are able to give a very good qualitative description of the in-plane boron vibrations in terms of the position of the Fermi level alone. Our study confirms the validity of the parabolic band model for the zone-center phonons and gives a simple explanation not only of the absence of renormalization of phonon frequencies, but also of the very small electron-phonon interaction at the zone edge and, thus, of the disappearance of any anharmonic effect.

Two-band Eliashberg model for MgB_2

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Abstract

We discuss a two-band strong-coupling model for superconductivity in MgB_2. The model is based on the results of first principle calculations of the electronic structure and the electron-phonon interaction in this material. The conditions of the validity and the limitations of the Eliashberg approach are discussed. The solutions of Eliashberg equations in both bands are discussed in Matsubara and real energy representations as a function of the interband impurity scattering rate. Critical temperature and gap distributions are compared within the four-band and two-band description of MgB_2. Several applications of the model are discussed:
(a) quasiparticle and Josephson tunneling in MgB_2-based junctions,
(b) the influence of the interband impurity scattering on the specific heat,

(c) the electromagnetic response in the far-infrared and microwave range. We discuss peculiarities in tunneling and microwave conductivity due to the interplay between the anisotropy of the transport coefficients and the pairing interaction in MgB_2.

Directional point-contact spectroscopy in MgB_2 and $Mg_{1-x}Al_xB_2$ single crystals: comparison to the predictions of the two-band model

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Abstract

There is a large consensus on the electron-phonon origin of superconductivity in MgB_2, and many recent experimental results from tunneling, point contact spectroscopy (PCS) and specific heat measurements have clearly shown the two-band character of superconductivity in this compound. In this framework it is of particular interest to compare the experimental results to the predictions of the two-band model regarding the temperature and magnetic-field dependencies of the gaps, the temperature dependency of the upper critical fields of the two bands and the dependency of the gaps on the doping in Al-doped samples. Here, we briefly summarize our recent results on the temperature dependency of Δ_σ and Δ_π obtained by directional point-contact spectroscopy on the surfaces, either parallel or perpendicular to the *ab* planes, of high-quality single crystals. The application of a proper magnetic field to our junctions (whose conductance curves clearly show Andreev-reflection features) allowed us to separate the contributions of the σ and π bands to the total conductance. Thus, we could determine with an unprecedented accuracy the temperature dependency of the gaps [1,2] that resulted in very good agreement with the prediction of the two-band model. By using the same technique, i.e. by applying magnetic fields up 9 T either parallel or perpendicular to the *ab* planes, we then performed the first PCS measurements of the upper critical fields of the σ and π bands of MgB_2 as function of temperature. For $T/T_c \lesssim 0.8$ the values we obtained (in both the $\mathbf{H} \parallel c$ and $\mathbf{H} \parallel ab$ configurations) are greater than the bulk H_{c2} (as measured by various techniques), but lower than the field that marks the onset of the superconducting transition. This unexpected result is probably connected to some surface effects, even though it cannot be simply explained in terms of nucleation of superconductivity on the surface at a field $H_{c3} > H_{c2}$. Finally, we used the aforementioned technique to study the gaps in Al-doped crystals. The results were found to be in clear contrast with the predictions of the two-band theory. At the increase of the Al content, both Δ_σ and Δ_π first strongly decrease and then, when $x = 25\%$, merge in a single small gap. In this situation, due to the rather large T_c of the junction, the ratio $2\Delta/k_BT_c$ is much smaller than the BCS value predicted by the two-band model in the dirty limit.

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[1] R.S. Gonnelli *et al.*, Phys. Rev. Lett. 89, 247004 (2002).
[2] D. Daghero *et al.*, Physica C 385, 255 (2003).

Enhancement of the upper critical field in the two-gap superconductor MgB_2 by selective tuning of impurity scattering

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Abstract

We report significant (3-10 fold) enhancement of the upper critical field H_{c2} of MgB_2 by doping with nonmagnetic impurities, which increases $H_{c2}(0)$ well above H_{c2} of competing non-cuprate superconductors like Nb_3Sn and Nb-Ti. Our high-field transport measurements gave $H_{c2}^{\perp}(0) \simeq 34$ Tesla and $H_{c2}\|(0) \simeq 49$Tesla for high resistivity ($\rho \sim 200\mu\Omega cm$) films and $H_{c2}(0) \simeq 29$ Tesla for untextured bulk polycrystals with $\rho \simeq 5 - 20\mu\Omega cm$. The observed $H_{c2}(T)$ exhibits a temperature dependent anisotropy and a strong upward curvature inconsistent with the standard dirty limit theory and the Ginzburg-Landau angular scaling. We show that both the significant enhancement of H_{c2} and its anomalous temperature dependence are consequences of the multiple scattering channels provided by the two-gap superconductivity in MgB_2 which offers special opportunities for further H_{c2} increase by tuning of the impurity scattering rates by selective alloying on Mg and B sites. We derived generalized Usadel equations for two-gap dirty superconductors and obtained an equation, which describes both the temperature dependence and the anisotropy of H_{c2}. The theory explains the observed anomalies of $H_{c2}(T)$ and shows that the significant enhancement of $H_{c2}(T)$ in the resistive film with the highest H_{c2} results from the stronger π-scattering due to disorder in the Mg sub-lattice. This conclusion was confirmed by transmission electron microscopy which shows noticeable buckling of Mg planes.

Phonons in MgB_2 and LiBC by polarized Raman scattering

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Abstract

We will present results on our recent Raman scattering investigations on few-micron size single-crystals of LiBC and MgB_2. Due to a natural hexagonal habitus of available crystallites, all components of the Raman tensor could be systematically investigated. In MgB_2, our polarized Raman experiments have shown that the strong and unusually broad band near

615 wavenumbers fully obeys the selection rules of E_{2g} phonon mode[1]. To shed a more light on the anharmonic nature of this unusual broadening, we have also investigated its temperature dependence. In the non-superconducting LiBC crystal, the corresponding B-C bond stretching modes do not show such a broadening[2]. Nevertheless, our measurements have revealed an unexpected lower symmetry modification of LiBC which can be converted to D_{6h} form by thermal annealing. All investigated crystals have been prepared and characterized by our collaborators from Institute od Electrical Engineering, SAS, Bratislava[1] and Institute fur Physik Universitat Augsburg, Germany[2].

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STM tunneling spectroscopy in MgB_2

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Abstract

A very peculiar feature of the recently discovered superconductor MgB_2 is the multigap nature of the superconducting state, which is now commonly accepted in the scientific community confirmed by a large number of experiments. The main issue in MgB_2 has been the existence of two distinct energy gaps, their effect on superconducting properties. Another important issue is the highly anisotropic MgB_2 band structure and its signature in different experiments. Tunneling spectroscopy is a powerful tool to directly probe the density of states on the surface and when it is combined with scanning capability it allows to study the detailed nature of superconductivity on a local scale. The highly anisotropic MgB_2 band structure acts as a momentum filter in a tunneling experiment, therefore the superconducting gap probed by Scanning Tunneling Spectroscopy should be momentum dependent. We report a systematic study of Scanning Tunneling Spectroscopy (STS) performed on high quality thin films, pellet and single crystals of MgB_2. Electron microscopy images and STM topography together with STS investigation allow direct correlation between tunneling direction and the observed tunneling spectra, confirming that the two-gap state is intrinsic to MgB_2. Tunneling along the c-axis we observe a single superconductive gap at ~ 3.2 meV, associated with the p band. Tunneling away from the c-axis the tunneling spectra dI/dV vs V clearly and consistently reveal double gap structure, flat background, and very low zero-bias conductance that is consistent with a little smearing other than thermal broadening. The first conductance peak is at ~ 3.2 meV and second one at ~ 7 meV, symmetrically for both injection and emission of electrons. The additional structure at ~ 7 meV originates from the highly 2D s-band. Magnetic field dependence of the spectra will also be presented and discussed as well as comparison between MgB_2 samples with different critical temperature T_c.

Andreev-reflection study in MgB_2

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Abstract

The energy-gap structure of MgB_2 is studied using the Andreev–reflection process in the ballistic charge-carrier transport across a normal-metal/superconductor interface. The measured current-voltage (I-V) characteristics of point contacts between MgB_2 and Cu reveal clear evidence for two-gap superconductivity in MgB_2 [1]. Depending on the direction of current injection on the probed crystallite, although of unknown orientation for the investigated polycrystalline samples, a single energy-gap structure or a two-gap structure are observed. The single small gap (gap ratio $2\Delta_S/k_BT_c = 1.3$) corresponds to current injection parallel to the c-axis probing the superconducting paring on the isotropic π-band. The additional large gap (gap ratio $2\Delta_L/k_BT_c = 4.0$) on the cylindrical σ-band part of the Fermi surface can be probed for an injection component parallel to the ab plane. Both energy gaps close near the same bulk critical temperature. In a magnetic field, pair breaking between the different bands can be distinguished. The small-gap structure is suppressed isotropically in a field of about 1.7 T. The large-gap structure is suppressed in a field of up to 15 T. In point-contact experiments on carbon-doped MgB_2 with a suppressed superconducting transition critical temperature $T_c = 22$ K we could only observe a single energy-gap structure closing at the bulk critical temperature. Like for the small gap in the pure system, the obtained gap ratio $2\Delta/k_BT_c = 1.7$ is strongly reduced compared to the BCS value. This gives an indirect indication that the two-gap structure is preserved in the carbon-doped samples.
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[2] P. Szabo et al., Supercond. Sci. Techn. **16**, 162 (2003).
[3] P. Samuely et al., cond-mat/0303644

Vortex studies in Magnesium Diboride

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Abstract

Recent results of vortex studies in MgB_2 are presented. Scanning tunneling spectroscopy (STS) was used to image vortices in pure MgB_2, tunneling both parallel and perpendicular to the c axis, as well as in aluminum-doped MgB_2, tunneling parallel to the c axis. Vortex imaging in pure MgB_2, with the tunneling current and field perpendicular to the c axis, revealed a distorted hexagonal vortex-lattice. The distortion is determined by the penetration

depth anisotropy, which is found to be much smaller than the upper critical field anisotropy. We also performed scanning tunneling spectroscopy of 2-3% aluminum-doped MgB_2. Tunneling parallel to the c axis, we are able to selectively measure the π band. In comparison to pure MgB_2, we find an increase of the superconducting gap from 2.2 meV to $\Delta_\pi = 2.64$ meV, and a decrease of the coherence length from 50 nm to $\xi_\pi \simeq 26$ nm. The increase of Δ_π and the decrease of ξ_π suggest that interband scattering is enhanced by Al-doping.
$\star$ In collaboration with G. Levy, M. Kugler, R. Cubitt, C. D. Dewhurst, J. Jun, S. M. Kazakov, J. Karpinski and Ø. Fischer.

Multiple gaps in MgB_2 and elsewhere: the information given by measurements of the specific heat versus magnetic field, orientation and disorder

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Abstract

Specific heat measurements using polycrystals and single crystals of MgB_2 have helped to establish the validity of the two-gap model in the bulk. We recall how zero-field data in the superconducting state reflect the distinct electronic excitation energies associated with these gaps, and how in-field data at $T << T_c$ can distinguish the contributions of each band owing to their different anisotropy. At variance with these results, disordering effects still remain to be explained, in part due to the added complication of different scattering channels. We present the continuation of our study of MgB_2 ceramics irradiated with neutrons, where T_c has now been suppressed down to 26 K. Bulk transitions remain well defined, in contrast to samples where disorder is obtained by chemical doping. The specific heat in the superconducting state still reflects an anomalous gap, which may be either multiple, or single but anisotropic. Increased scattering leads to an increase of the upper critical field. We also present preliminary results on Nb_3Sn, showing similar, but weaker effects.

Experimental evidence of two-band behavior of MgB_2

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Abstract

In the present investigation the current-voltage characteristics (CVC) of more than 150 break-junctions in polycrystalline MgB_2 samples have been studied in the temperature range $4.2\ \mathrm{K} < T < T_c$. The break-junction technique allows changing the junction properties during the measurements, so that the tunnel contact like (SIS) and point contact like (SNS) behavior could be investigated on the same sample. We have found that the temperature dependence of a large gap Δ_L is qualitatively close to the BCS type but the ratio $2\Delta_L/kT_c = 5.3$ surpasses the BCS value: 3.52. The temperature dependence of a small gap Δ_S can be different for different junctions. In all cases $\Delta_S(T)$ deviates significantly from the BCS type behavior which could be the result of the 'intrinsic proximity' effect ('proximity' effect in k-space). However, both gaps close at one and the same critical temperature T_c. While investigating SNS contacts with different local T_c we have found that only a big 2D gap Δ_L scaled with T_c. At the same time a small 3D gap Δ_S showed no reasonable tendency to change in the range $25\ \mathrm{K} < T_c < 40.5\ \mathrm{K}$. We have observed CVCs of stacks of SIS and SNS Andreev junctions. We believe that this effect is similar to that observed in high-T_c superconducting cuprates and is related to the layered structure of MgB_2 and to the existence in boron planes of two-dimensional sigma-bands which have a weak interband coupling with three-dimensional pi-bands. It shoud be noted that an observation of two-gap structures in the CVCs of stacks of SIS or SNS contacts proves a two-gap superconductivity to be an essentially intrinsic property of MgB_2. We have found that the typical values of a characteristic voltage $V_c = I_c R_n$ for the investigated MgB_2 Josephson junctions lie within the range 3.0 — 6.0 mV. This result supports indirectly the validity of the two-gap model for MgB_2. Multi-band superconductors can possess some special collective excitations due to different values of the order parameter phases in different bands. The existence of such collective modes has been predicted by Leggett. We have clearly observed the manifestation of this mode with the energy $\Omega_0 \sim 4$ meV in the CVCs of Josephson junctions and SNS-contacts at $T < T_c$.

The Phase - Slip Centers in the MgB_2 wires

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Abstract

High-density MgB_2 superconducting wires were produced by reacting Boron filaments with the vapor of very pure Magnesium metal. We characterized the morphology of the wires by STM microscopy and its composition by EDAX and XRD spectroscopy. The critical currents and fields were measured in four points transport experiments. Magnetizations vs. field and vs. temperature were obtained in a SQUID magnetometer. The most interesting finding, which emerged from the above measurement, is the observation of phase - slip centers in the wires. When at certain location in the filament the critical current is somewhat smaller than elsewhere, an increase in current will bring this point to its normal state - causing normal flow of electrons through this weak point. This flow will induce an electric field. The latter, in turn, will accelerate the normal electrons to the critical velocity. Electron pairs at the weak spot will be broken, the amplitude of the order parameters $|\Psi|$ will go to zero and

the current will be carried by the normal component only. But at low enough temperatures the formation of electron pairs is favored. Therefore, the amplitude of the order parameters $|\Psi|$ will become nonzero again and the current will be carried partly by S.C. electrons i.e. super current will appear. Then the entire process will repeat itself. On completion of each cycle, the phase difference of the S.C. electron wave functions to the left and to the right of the weak spot will vary by 2π, so called phase slip center. The size of the center, δ, is the region in which oscillations of $|\Psi|$ take place, $\delta \approx 2\xi(T)$, where ξ is the correlation length. Experimentally the phase slip process is distinguished by a staircase response in current - voltage characteristics. This response can be interpreted in view of the granular structure that is observed in the MgB_2 high-density filaments.

Phonon and electron-phonon renormalization in Al doped MgB_2

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Abstract

We report a detailed ab-initio study of the electronic properties of the Al doped $MgAlB_2$ compound. In particular, we show how the E_{2g} phonon frequency evolves as a function of the Al content within Linear Response theory, using the virtual crystal approximation. Our results show that a strong phonon frequency renormalization starts at 25% Al content, explaining the phonon frequency behaviour as a function of Al doping reported by different experiments. Our results will be used to investigate the delicate interplay between electronic structure and superconducting properties in this system.

The electronic properties of C-subsituted MgB_2 single crystals

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Abstract

We have recently succeeded in growing single crystal MgB_2 with carbon substitution as much as 12 %. The superconducting transition temperature is drastically suppressed by the carbon substitution. Increases of H_{c2} were observed in modelately substituted crystals in both H//c and H//ab directions. I will also show the resistivity, Hall coefficient, Raman scattering results and discuss the effect of carbon substitution on the electronic properties of MgB_2.

This work was supported by the New Energy and Industrial Technology Development Organization (NEDO) as Collaborative Research and Development of Fundamental Technologies for Superconductivity Applications.

Role of anharmonicity in phonon frequencies and lifetimes of MgB_2

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Abstract

We compute the anharmonic contributions to the phonon self-energy for MgB_2. We consider all the lowest order terms from three- and four-phonon vertices. The scattering between different phonon modes at different k-points in the Brillouin zone are included. We use density functional theory and the (2n+1) theorem to evaluate the three- and four-phonon vertices. We extract anharmonic phonon frequency shifts and linewidths (the inverses of the lifetime) at Gamma, A, M from the real and imaginary part of the phonon self-energy. We find the anharmonic linewidth of the E_{2g} mode to be negligible compared to that due to electron-phonon coupling [1]. Thus the measurement of the phonon linewidths allows the experimental determination of the electron-phonon couplings. For the frequency shift, we find a cancellation between the contributions of the three- and four-phonon vertices [2]. The total anharmonic shift of the E_{2g} mode at Gamma is +3.5 meV, corresponding to a relative frequency shift of +5.4%. The resulting anharmonic phonon frequencies are in good agreement with the phonon dispersion measured with inelastic X-ray scattering [1].
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[2] M. Lazzeri, M. Calandra, F. Mauri to be published.

An overview of the theory of superconductivity in MgB_2

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Abstract

I will briefly review the story of the theoretical efforts to understand superconductivity in MgB_2 and the remaining theoretical challenges. A unique side of this story is that the theory, mostly the ab initio computational theory, largely let the whole field, with major prediction later confirmed by the experiment, namely
(1) exclusive role of the boron p-states, with the consequence of a sizeable B isotope effect and negligible Mg isotope effect and

(2) two-gap character of superconductivity. As a result, there is now the consensus that MgB_2 is an intermediate-coupling Eliashberg-type superconductor, with most of the coupling coming from interaction of just two strongly anharmonic phonons at the zone center with two out of four bands, and that there are two very different gaps for the two sets of bands, which are surprisingly robust to various defects. This was confirmed by various experiments. However, there are still several open questions, even puzzles, that wait for solutions. These include some normal transport properties, issues of the impurities effect on superconductivity, as well as some quantitative aspects of the existing first principles calculations.

Theory of normal state NMR in $Mg_{1-x}Al_xB_2$

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Abstract

We have performed[1-3] ab-initio calculations of the nuclear magnetic resonance (NMR) Knight shifts (K) and relaxation rates ($1/T_1T$) in $Mg_{1-x}Al_xB_2$. The comparison with NMR experimental results allows us to extract reliable information on the electronic structure. In the case of ^{11}B NMR, we find that for small x the dominant relaxation mechanism is the interaction of the nuclear spin with the electronic orbital moment. For large x the situation changes drastically, the ^{11}B relaxation mechanism becoming mostly the Fermi contact interaction. This is caused by the filling of the B p_σ bands: while they are partially filled in MgB_2 ($x = 0$) they are completely occupied in AlB_2 ($x = 1$) and thus do not contribute to the orbital term. Taking the Stoner enhancement, which we have calculated *ab-initio*, into account, very good agreement with experimental data is found. Both experimental and theoretical results show[2,3] that in AlB_2 the density of states in the B plane is strongly reduced with respect to MgB_2. In the case of ^{27}Al and ^{25}Mg relaxation, we find that the dominant mechanism is the Fermi contact interaction, which also dominates the ^{27}Al and ^{25}Mg Knight shifts. This result holds for all values of x. The dependence upon Al doping is fairly well reproduced for all considered nuclei, and for both K and $1/T_1T$. However, surprisingly the calculated ^{27}Al Korringa ratio $R = 1/T_1TK^2$ is a factor of 2 smaller than recently reported experimental estimates[3]. Consequences concerning the electronic structure of $Mg_{1-x}Al_xB_2$ are discussed.

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[3] S. Serventi et al., submitted to Phys. Rev. B.

Alloying, strain, and extreme electron-phonon coupling in the MgB_2 class of superconductors

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Abstract

The discovery of superconductivity at 40 K in the intermetallic compound MgB_2, which has no *d* electrons, no peak at the Fermi level, is not cubic, and therefore "should not" be a good intermetallic superconductor, has reinvigorated superconductivity research. Many of the answers to questions raised by this compound have already been answered by the combined efforts of several groups. This talk will focus on new results in the following areas.
(1) Other materials in the *MgB_2-class*: hole-doped LiBC and MgB_2C_2 – can they be expected to be good superconductors? $Li_{1-x}BC$ should be an excellent superconductor, but it has proven difficult so far to extract Li. We argue that MgB_2C_2 also is an excellent candidate.
(2) Strained MgB_2 films: a recent report by Pogrebnyakov *et al.* (cond-mat/0304164) has confirmed the previous report of Hur *et al.*[Appl. Phys. Lett. **79**, 4180 (2001)] that strain in MgB_2 films can raise T_c by nearly 5%, to $T_c \approx 41.8$ K. We report the calculated effects of strain on the σ-hole density and assess the probable cause of the observed increase in T_c.
(3) Doping of C onto the B sites in MgB_2 is possible up to about 10%, decreasing the value of T_c to near 20 K. We report the calculated effects of B replacement by C. We find that (i) rigid band treatment of C alloying is not sufficiently accurate, and (ii) there are still enough σ band holes in $Mg(B_{0.9}C_{0.1})_2$ to be consistent with the observed T_c.
(4) $T_c \approx 40$ K in MgB_2 results from extremely strong coupling of the σ-type holes to the bond stretching modes, as revealed by several groups. We reassess this extreme electron-phonon coupling, show that the two-dimensionality of the σ bands leads to unexpected behavior of T_c versus carrier concentration, and display and analyze the colossal Kohn anomalies at $2k_F$. We also argue that Migdal-Eliashberg theory for el-ph coupling in MgB_2 has no validity, and that the strongly coupled σ hole – bond-stretching mode system forms a *dynamical soup* that demands an extension of the theory.
Supported by the National Science Foundation.

Raman investigation of $Mg_{(1-x)}Al_xB_2$: effects of Al content and pressure on the phonon spectra

P. Postorino
Rome, Italy

Abstract

An extended investigation of the Al-substituted MgB_2 samples has been carried out by means of optical spectroscopy techniques. In particular Raman spectra of polycrystalline samples of $Mg_{(1-x)}Al_xB_2$ with the Al concentration ranging from 0 to 0.5, have been collected at ambient pressure and room temperature. The spectra show a remarkable x-dependence, and a systematic narrowing of the Raman-active phonon modes is well evident with increasing x. The data analysis, and in particular the x-dependence of the phonon

frequencies, widths and intensities, allow us to distinguish between two regimes of low and high Al content regions. A connection between the whole of our results and the suppression of the superconducting phase at high Al content is suggested and discussed. Finally latest Raman data on $Mg_{0.5}Al_{0.5}B_2$, collected by using the diamond anvil cell technique over the 0-12 GPa pressure range, and Raman data on three $Mg_{(1-x)}Al_xB_2$ compounds (x=0, 0.33, 0.5) exploiting the isotopic substitution of Boron are presented. A critical discussion and comparison of the present data with those of literature are given.

The effect of disorder and doping on gap amplitudes and relaxation rates of σ and π bands

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3-INFM-NRC S, Dipartimento di Fisica, via G.Campi 213/A, I-41100 Modena, Italy.

Abstract

We present thermal conductivity and specific heat measurements on MgB_2 in order to study the dependence on the disorder and doping of gap amplitudes and relaxation rates of π and σ bands. The transport properties are performed on bulk samples obtained by an one step technique which provides very clean poly-crystals with well connected grains as indicated by residual resistivity values as low as 0.5 mW cm and thermal conductivity values higher than 200 W/mK. Starting from the purest samples the disorder were introduced by chemical substitution or by irradiation. Specific heat measurements are performed on poly-crystalline Mg-AlB_2 samples. Thermal properties have been analyzed by using a two-gap model in order to estimate the gap amplitudes, $\Delta(0)_\pi$ and $\Delta(0)_\sigma$ and the intra-band scattering rates for scattering with impurity, $\Gamma_{\sigma\sigma}$ and $\Gamma_{\pi\pi}$. $\Delta(0)_\pi$ and $\Delta(0)_\sigma$ have been analyzed as a function of disorder and Al doping; in both the cases $\Delta(0)_\sigma$ rapidly decreases, while $\Delta(0)_\pi$ is found to be nearly constant. $\Gamma_{\sigma\sigma}$ and $\Gamma_{\pi\pi}$ can be estimated by thermal conductivity; they increase as the disorder increases , being $\Gamma_{\pi\pi}$ more affected than $\Gamma_{\sigma\sigma}$. An evaluation of the inter-band relaxation time $\Gamma_{\sigma\pi}$ can be given by the T_c suppression in disordered samples. In all the samples we find $\Gamma_{\sigma\pi} \ll \Gamma_{\sigma\sigma}, \Gamma_{\pi\pi}$.

Two-gap interplay in MgB_2 : a tunneling spectroscopy study

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4-Laboratoire de Cristallographie et LEPES, CNRS, Grenoble,France

Abstract

Tunneling spectroscopy of thin films and clusters of MgB_2 was performed at low temperature using STM/STS. The experiments performed on clusters in the standard N-I-S geometry evidenced for two strongly coupled gaps $\Delta_L = 7.0 \pm 1.0$ meV and $\Delta_S = 3.0 \pm 1.0$ meV at 4.2 K. This technique allowed to show that both gaps close at the critical temperature of the bulk material but have different temperature dependencies. STS on as-grown c-axis oriented thin films yielded only small gap which confirmed the identification of this gap as originating from 3D-like π-band and, by exclusion, that of the large gap from 2D-like σ-band. The low gap values $\Delta_S = 2.2 \pm 0.3$ meV were attributed to the degraded film surface. After chemical etching, the gap increased to $\Delta_S = 2.8 \pm 0.3$ meV. Tunneling spectroscopy on thin films was performed also in SIS geometry by gently crashing the Pt/Ir tip into the film surface and attaching in this way a small cluster of MgB_2 to the tip. In such a SIS geometry the tunneling takes place from both π- and σ-bands of the cluster to the π-band of the c-oriented film. The SIS spectroscopic features in these tunneling spectra are much more pronounced as compared to the SIN case, allowing a more detailed analysis. The temperature and magnetic field dependencies of apparent superconducting gap energies were extensively studied. Neither $\Delta_S(B)$ nor $\Delta_S(T)$ appear conventional. The observed behaviour is discussed in terms of two-gap superconductivity in the presence of inhomogeneities and (or) surface states.

Electronic properties of MgB_2

H. Romdhani

Laboratoire de physique de la matière condensé
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Abstract

The recent discovery of superconductivity with high T_c in MgB_2 has initiated a large experimental and theoretical activity. Within the local-density approximation, using the relativistic full-potential linearised augmented plane wave (FLAPW) method, the band structure is calculated for the layered material MgB_2. Total and partial densities of states were calculated and used to give an interpretation of the chemical bonding. The resulting high density of p boron states at the Fermi level and the existence of $p_{x,y}$ holes are believed to contribute to the high T_c of MgB_2 compound. The inclusion of spin-orbit coupling has no effect on the change of electronic properties. The ground-state calculation was repeated

using the Stuttgart tight-binding linear muffin-tin orbital method in the atomic sphere approximation (TB.LMTO-ASA), and the resulting band structure agree very well with the FLAPW method.

Superconductivity in MgB_2 and $MgCNi_3$: two opposite cases

S.Y. Savrasov
New Jersey Institute of Technology, Newark, USA

Abstract

In this talk I will discuss the calculations of lattice dynamical properties and strength of the electron-phonon coupling in $MgCNi_3$. Phonons contributing to lambda will be emphasized, and superconductivity will be compared to the case of MgB_2.

Disorder effects in MgB_2 using SIS tunneling spectroscopy

H. Schmidt,* K.E. Gray, J.F. Zasadzinksi,* D.G. Hinks, M. Avdeev,
J.D. Jorgensen, and J.C. Burley
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Abstract

Break–junction tunneling spectroscopy is used to study the effect of disorder on the size and spectral shape of the two energy gaps in MgB_2. Samples used are polycrystalline pellets that predominantly show clean behavior, $T_c \sim 39$ K and $\Delta_\pi \sim 2.5$ meV. A small fraction of the data exhibit a reduced critical temperature $T_c \sim 30$ K and proportionately smaller gap values. Also, the critical temperature was intentionally decreased by heavy C–doping, resulting in $T_c \sim 22$ K and $\Delta_\pi \sim 1.5$ meV. Thus two–band superconductivity is found to survive in all cases of reduced superconductivity and we conclude that interband scattering is not affected by either native disorder or heavy C–doping. The interband quasiparticle scattering feature we see in the π–band density of states is successfully fit using McMillan's model of the proximity effect, however, this interband quasiparticle scattering presumably is not due to disorder. No evidence is found that these features are enhanced in C–doped MgB_2 consistent with the absence of an increase in interband scattering.

Thermal conductivity of MgB_2 and multigap superconductivity

A.V. Sologubenko and H.R. Ott
Laboratorium für Festkörperphysik, ETH Hönggerberg, Zürich, Switzerland

Abstract

Measurements of the thermal conductivity in MgB_2 in the region of T_c and below have revealed anomalous temperature and field dependences of the heat transport in the superconducting phase of this material, which are very difficult to explain in terms of a single order parameter, even when considering its possible anisotropy. In particular, a very fast increase of the electronic thermal conductivity with increasing external magnetic field at low temperatures is unprecedented for other, both conventional and unconventional, superconductors, but finds a natural explanation by considering the electronic heat transport to occur via two weakly interacting groups of quasiparticles with distinctly different energy gaps in their excitation spectra. Recent theoretical calculations of the electronic heat transport in two-gap superconductors support this interpretation of the experimental data. The analysis of thermal conductivity data in the mixed state provides valuable information about the relative strengths of defect scattering in different energy bands, as well as about the interband scattering processes. More recent observations of heat transport anomalies in $NbSe_2$, another superconductor with claimed multigap features, are also presented and discussed.

4 News from UK's CCP9 Programme

UK's Collaborative Computational Project 9 on "Computational Studies of the Electronic Structure of Solids"

4.1 Reports on CCP9 Workshops

4.1.1 Report on "International Workshop on the Bogoliubov de Gennes Equations for Superfluids"

CCP9 and Ψ_k network Workshop:

"International Workshop on the Bogoliubov de Gennes Equations for Superfliuds"

Burwalls Centre
University of Bristol,
Bristol, UK
May 30 - June 1, 2003

The **"International Workshop on the Bogoliubov de Gennes Equations for Superfliuds "** was held in Bristol over the weekend 30 May- 1 June 2003. The topics covered included applications of the Bogoliubov de Gennes (BdeG) equations to: bulk superconductors, mesoscopic superconductors, Josephson junctions, vortex matter, semiclassical transport theories, and Bose-Einstein condensates. The BdeG equations form a common theoretical framework under which all of these diverse topics in superconductivity and superfluidity can be addressed.

Several talks concerned pairingand transport in mesoscopic superconductors. The talks by V. Falko and M. Krawiec concerned the proximity effect and transport in mesoscopic structures containing both superconducting and ferromagnetic elements. The spin accumulation and spontaneous spin polarized currents predicted for these structures provide interesting novel opportunities for spin manipulation, spin injection and spintronics. M. Eschrig showed that the induced

p-wave Cooper pairing near a S/N interface leads to an unusual long-ranged Josephson effect in superconductor-half metal-superconductor trilayers. Other talks on transport concerned weak localization effects at S/F interfaces (McCann) and the fluctuation corrections to thermal conductivity (Smith). Tanaka addressed the electronic states in the presence of superconducting vortices in mesoscopic systems, and Quintanilla discussed anomalous Josephson effects in high T_c superconductor junctions.

The theme of semiclassical methods for transport was developed in talks by Gyorffy, Sieber, Cserti and Polniak. Sieber outlined a general theory for quantum transport in chaotic systems, while Gyorffy and Cserti considered the formulation of semiclassical approximations for quasiparticle states in superconductors.

The boson or superfluid analogue of the fermionic Bogoliubov de Gennes equations are the Gross-Pitaevskii equations. The solutions of these equations lead to a number of effects in superfluids and in Bose-Einstein Condensates (BEC). Ruostekoski and Martin discussed the solution of these equations, especially in the presence of periodic optical lattice potentials.

A series of talks on novel superconducting materials included talks on high T_c superconductors (Hussey), $ZrZn_2$ (Santi), Sr_2RuO_4 (Litak) and MgB_2 (Gabovich). Hussey presented dramatic new experimental evidence for a fully three dimensionl Fermi surface in the cuprate superconductors, which is in good agreement with band theory predictions. Santi showed that LSDA band calculations give a good basis for understanding both the static ferromagnetism in the weak itinerant magnet $ZrZn_2$, and that the spin fluctuations about this ground state provide a possible route towards understanding the superconductivity in this material. Litak presented a model for the exotic material Sr_2RuO_4, corresponding to a unique p-wave pairing state, analogous to the A phase of suerfluid ^{4}He. Finally, Gabovich argued that the miutiband models of superconductivity in MgB_2 are not consistent with experiments, and instead result from a spatially inhomgenous distribution of local gap values.

A relatively new theme is the application of superconducting devices for possible applications in quantum computing and quantum information. This area was reviewed by Annett, who also discussed the possibility of observing entanglement between two macroscopic superconducting devices. Vourdras considered the further effects that can occur in such superconducting quantum coherent devices when the quantization of external microwave fields is taken into account.

Finally, Moradian presented new results on the density of states for a Ni impurity in a BSCCO high T_c superconductor, and its comparison to recent STM experiments by Davis et al..

James F Annett and Balazs L Gyorffy

List of Participants

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Friday, May 30th, 2003

19.00 – 20.00 **Arrival and Registration**

Saturday, May 31st, 2003

09.00 – 09.30 **V. Falco** (Lancaster),
Subgap Transport Spin Accumulation and Relaxation in SF Junctions

09.30 – 10.00 **M. Krawiec** (Bristol),
Current Carrying Ground States of S/F Structures

10.00 – 10.30 **M. Eschrig** (Karlsruhe),
P-wave Pairing at S/N Interfaces

10.30 – 11.00 **G Tkachov** (Lancaster),
Thermal Conductance of a Proximity Effect SN System in a Magnetic field

11.00 – 11.30 coffee

11.30 – 12.00 **E. McCann** (Lancaster),
Weak Localization Correction to S/F Contact Resistance

12.00 – 12.30 **K. Tanaka** (Saskatchewan),
Electronic Structure of Mesoscopic Vortex Matter

12.30 – 13.00 **R. Smith** (Birmingham),
Absence of Singular Superconducting Fluctuation Correction to Thermal Conductivity

13.00 – 14.00 lunch

14.00 – 14.30 **J. Quintanilla** (Birmingham),
Anomalous Proximity Effects in High T_c Josephson Junctions .....

14.30 – 15.00 **J. Cserti** (Budapest),
A Semiclassical Approximation for QuasiParticles in Superconductors

15.00 – 15.30 **P. Polniak** (Lancaster),
Ring Shaped Andreev Billiards in Quantizing Magnetic Fields with both surface and on-site disorder

15.30 – 16.00 **B. Gyorffy** (Bristol),
Semiclassics for Quasi Particles in the Superconducting State

16.00 – 16.30 **M. Sieber** (Bristol),
Semiclassical Theory of Chaotic Quantum Transport

16.30 – 17.00 coffee

17.00 – 17.30 **J. Ruostekoski** (Hertfordshire),
Bose-Einstein Condensation of Atoms

17.30 – 18.00 **A. Martin** (Nottingham),
Bragg Reflections of Dilute Bose Gas Condensates

Sunday, June 1st, 2003

09.00 – 09.30	**N.E. Husey** (Bristol), The Fermi Surface of High Temperature Superconductors as revealed by Angular Magnetoresistance Oscillations
09.40 – 10.00	**G. Santi** (Bristol), Magnetic and Superconducting Properties of $ZrZn_2$ from Ab Initio Calculations
10.00 – 10.30	**G. Litak** (Lublin), Triplet Pairing in Strontium Ruthenate
10.30 – 11.00	**A. Gabovich** (Kiev), MgB_2 How Many Gaps?
11.00 – 11.30	coffee
11.30 – 12.00	**J.F. Annett** (Bristol), Quantum Computing with Small superconductors
12.00 – 12.30	**A. Vourdras** (Bradford), Vortices in Josephson array insulators interacting with non-classical microwaves
12.30 – 13.00	**R. Moradian** (Kermanshah), Effects of Random Hopping Integrals on Disordered D-Wave Superconductors
13.00 – 14.00	lunch and close

Abstracts

Subgap Transport Spin Accumulation and Relaxation in SF Junctions

Vladimir I. Fal'ko

Department of Physics, Lancaster University,
Lancaster, LA1 4YB, United Kingdom

Abstract

It is shown that the mismatch betwen spin-polarised electron current in a ferromagnet and spinless current in a superconductor generates an additional contact resistance in SF junctions for $eV < \Delta$. The value of such resistance depends on the spin relaxation length of electrons in a ferromagnetic metal. We also found that magnon emission assisted Andreev reflection opens an additional channel for the sugbap transport in SF junctions, giving rise to the non-linear and asymmetric contribution to the $I(V)$ charactersitics which depends on the density of magnon states in the ferromagnet.

Current Carrying Ground States of S/F Structures

M. Krawiec, B.L. Gyorffy and J.F. Annett

HH Wills Physics Laboratory, University of Bristol,
Royal Fort, Tyndall Avenue, Bristol BS8 1TL, United Kingdom

Abstract

We study the ground state properties of a ferromagnet-superconductor heterostructure on the basis of a quasiclassical theory. We have solved the Eilenberger equations together with Maxwell's equation fully self-consistently and found that due to the proximity effect a Fulde-Ferrel-Larkin-Ovchinnikov (FFLO) like state is realized in such system. Moreover this state has oscillations of the pairing amplitude in either one or two directions, depending on the exchange splitting and thickness of the ferromagnet. In particular, using semiclassical arguments (Bohr-Sommerfeld quantization rule) we show that owing to the presence of the Andreev bound states in the ferromagnet, a spontaneous current in the ground state is generated as a hallmark of the FFLO state in the direction parallel to the interface. We also discuss the effects of the the elastic disorder and finite transparency of the interface on the properties of the *FFLO* state in the system.

P-wave Pairing at S/N Interfaces

M. Eschrig

Institut fuer Theoretische Festkoerperphysik Universitaet Karlsruhe, D-76128 Karlsruhe, Germany

Abstract

We introduce the indirect proximity effect between a superconductor and a half metal via triplet correlations on the superconducting side of the interface. We present a theory appropriate for studying this phenomenon and apply it to study the resulting indirect Josephson effect in a superconductor/half metal/superconductor heterostructure.

Thermal Conductance of a Proximity Effect SN System in a Magnetic field

Grigory Tkachov

Department of Physics, Lancaster University,
Lancaster, LA1 4YB, United Kingdom

Abstract

We show that magneto-tunnelling of Cooper pairs from a superconductor to a ballistic quasi-one-dimensional (Q1D) electron channel results in the shift of a minigap in the excitation spectrum of the Q1D system from the Fermi level to higher energies. The thermal conductance of the channel normalized by that of a normal Q1D ballistic system is predicted to exhibit a pronounced minimum at the temperatures corresponding to the gapful part of the spectrum.

Weak localization correction to the ferromagnet-superconductor interface resistance

Edward McCann, Vladimir I. Fal'ko, A. F. Volkov, and C. J. Lambert

Department of Physics, Lancaster University,
Lancaster, LA1 4YB, United Kingdom

Abstract

The classical resistance of a contact between a ferromagnet (F) and a superconductor (S) acquires an additional contact term as compared to the contact between a ferromagnet and a normal metal. The necessity to match spin-polarized current in a ferromagnet to spin-less current in the superconductor results in the accumulation of non-equilibrium polarization near the F/S interface. In the present work, we show that the weak localization correction to the classical diffusion coefficient, δD, is dependent on the degree of polarization, with majority spins more likely to be reflected from the interface than minority spins. Taking into account the change in the spin polarized particle distribution in the F wire arising from δD, we calculate the weak localization correction to the F/S contact resistance.

Electronic Structure of Mesoscopic Vortex Matter

K. Tanaka

University of Saskatchewan, Physics and Engineering Physics, 116 Science Place, Saskatoon, Saskatchewan, Canada

Abstract

We study the electronic structure of giant vortex states in a mesoscopic superconductor in terms of the Bogoliubov-de Gennes formalism, and examine the effects of quantum confinement and surfaces.

Absence of Singular Superconducting Fluctuation Correction to Thermal Conductivity

R. Smith

School of Physics and Astronomy, University of Birmingham, Birmingham, B15 2TT, United Kingdom

Abstract

We evaluate the superconducting fluctuation corrections to thermal conductivity in the normal state which diverge as T approaches T_c. We find zero total contribution for one, two and three-dimensional superconductors for arbitrary impurity concentration. The method used is diagrammatic many-body theory, and all contributions – Aslamazov-Larkin (AL), Maki-Thompson (MT), and density-of-states (DOS) – are considered. The AL contribution is convergent, whilst the divergences of the DOS and MT diagrams exactly cancel.

Anomalous Proximity Effects in High T_c Josephson Junctions

J. Quintanilla

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Abstract

In an interesting photo-doping experiment Decca et al. [PRL 85, 3708 (2000)] observed an unusually long-ranged proximity effect between the superconducting and insulating phases of YBCO. It was claimed that such long range was an unconventional property of high-temperature superconductors and, on the basis of this, several interpretations were put forward [Wand and Balatsky, PRB (2001); Kwon, PRB (2001); Burgy et al., PRL (2001)]. More recently, we have critically examined the original claim that such long range is anomalous [PRL 90, 089703 (2003)]. I shall describe how, once the novel nature of the experiments has been properly accounted for, even the conventional theory of the proximity effect predicts comparably long ranges. In this view, the long range is a signature of critical opalescence, which becomes observable only thanks to the delicate way in which photodoping allows the tuning of the material's parameters.

A Semiclassical Approximation for QuasiParticles in Superconductors

J. Cserti

Department of Physics of Complex Systems, Eotvos University, H-1117 Budapest, Pazmany Peter Setany 1/A, Hungary

Abstract

We have calculated energy levels of the so-called Andreev billiards consisting of a superconductor attached to a normal dot by using exact and semi-classical treatment. Recent studies show that the energy spectrum of the Andreev billiards are gapless if the normal dot is classically integrable whereas there is a sub gap for chaotic dots. We have studied several Andreev billiards (integarble, pseudo-integrable and chaotic) and shown that the density of states obtained from semi-classics are in very good agreement with the exact results. It is shown that for pseudo-integrable case there is a sub gap in contrast to earlier predictions and its value can be much larger than that predicted for chaotic case.

Ring Shaped Andreev Billiards in Quantizing Magnetic Fields with both surface and on-site disorder

P. Polniak

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Semiclassics for Quasi Particles in the Superconducting State

B. Gyorffy* and K.P. Duncan**

* *H.H. Wills Physics Laboratory, University of Bristol, Royal fort, Tyndall Avenue, Bristol BS8 1TL, United Kingdom*

** The Open University, Milton Keynes, MK7 6AA, United Kingdom

Abstract

The case for developing a semiclassical approach to solving the Bogoliubov-de Gennes equation is argued and a methodology for doing so is developed. It is based on the study of semiclassical orbits which have both particle and hole like segments and are governed by an effective Hamiltonian describing quasiparticles in the superconducting state. It includes an account of the appropriate generalization of torus quantization,the Bohr- Sommerfeld quantiasation rules, Maslov indices, topological phases arising from lines of phase singularities of the order parameter field (vortices) and semiclassical wavefunctions for multidimensional systems. The method is illustrated by treatments of S/N/S junctions, a single vortex, and the Abrikosov flux lattice.

Semiclassical Theory of Chaotic Quantum Transport

M. Sieber[1], K. Richter[2]

[1] *Department of Mathematics, University of Bristol, Royal fort, Tyndall Avenue, Bristol BS8 1TL, United Kingdom*

[2] *Univ Regensburg, Inst Theoret Phys, D-93040 Regensburg, Germany*

Abstract

The conductance through a clean chaotic cavity is evaluated in the semiclassical approximation. A weak-localization correction is obtained in agreement with results from random matrix theory by including off-diagonal contributions to double sums over classical paths.

Bose-Einstein Condensation of Atoms

J. Ruostekoski

Department of Physical Sciences, University of Hertfordshire, Hatfield, Herts AL10 9AB, United Kingdom

Abstract

The observation of the Bose-Einstein condensation in dilute alkali-metal atomic gases represents a major breakthrough in AMO physics. Bose-Einstein condensates form a coherent source of atoms analogous to optical lasers. Moreover, the condensates can exhibit stable particle-like topological solitons with a strong analogy to cosmic vortons and vacuum states encountered in modern relativistic quantum field theories.

Bragg Reflections of Dilute Bose Gas Condensates

A. Martin

School of Physics and Astronomy, University of Nottingham, University Park, NOTTINGHAM, NG7 2RD United Kingdom

Abstract

We study the dynamics of Bose-Einstein condensates in an optical lattice and harmonic trap. The condensates are set in motion by displacing the trap and initially follow simple semiclassical paths, shaped by the lowest energy band. Above a critical displacement, the condensate undergoes Bragg reflection. For high atom densities, the first Bragg reflection generates a train of solitons and vortices, which destabilize the condensate and trigger explosive expansion. At lower densities, soliton and vortex formation requires multiple Bragg reflections, and damps the center-of-mass motion.

The Fermi Surface of High Temperature Superconductors as revealed by Angular Magnetoresistance Oscillations

N.E. Husey

H.H. Wills Physics Laboratory, University of Bristol, Royal fort, Tyndall Avenue, Bristol BS8 1TL, United Kingdom United Kingdom

Abstract

We report the observation of polar angular magnetoresistance oscillations in the high-T_c cuprate $Tl_2Ba_2CuO_6$ in high magnetic fields up to 45 Tesla. These measurements establish the existence of a coherent three-dimensional Fermi surface on the overdoped, superconducting side of the cuprate phase diagram, even in materials with extreme electrical anisotropy. Detailed analysis of the oscillations however reveals that c-axis dispersion vanishes at specific symmetry points. The possible implications of this finding for our understanding of a wide range of unusual metallic and superconducting properties of these ground-breaking materials will be discussed.

Magnetic and Superconducting Properties of $ZrZn_2$ from Ab Initio Calculations

G. Santi[1], S.B. Dugdale[1], T. Jarlborg[2]

[1] *H.H. Wills Physics Laboratory, University of Bristol, Royal fort, Tyndall Avenue, Bristol BS8 1TL, United Kingdom*

[2] *Univ Geneva, Dept Phys Mat Condensee, CH-1211 Geneva 4, Switzerland*

Abstract

The recent discovery of superconductivity coexisting with weak itinerant ferromagnetism in the d-electron intermetallic compound ZrZn2 strongly suggests spin-fluctuation mediated superconductivity. Ab initio electronic structure calculations of the Fermi surface and generalized susceptibilities are performed to investigate the viability of longitudinal spin-fluctuation-induced spin-triplet superconductivity in the ferromagnetic state. The critical temperature is estimated to be of the order of 1 K. Additionally, it is shown that in spite of a strong electron-phonon coupling (lambda (ph) = 0.7), conventional s-wave superconductivity is inhibited by the presence of strong spin fluctuations.

Triplet Pairing in Strontium Ruthenate

G.Litak[1], J.F. Annett[2] B.L. Gyorffy[2], and K.I. Wysokinski[3]

[1] *Department of Mechanics, Technical University of Lublin, Nadbystrzycka 36, 20-618 Lublin, Poland.*

[2] *H.H. Wills Physics Laboratory, University of Bristol, Royal fort, Tyndall Avenue, Bristol BS8 1TL, United Kingdom*

[3] *Institute of Physics, M. Curie-Skłodowska University, Radziszewskiego 10, 20-031 Lublin, Poland*

Abstract

We study the superconducting state of Sr_2RuO_4 on the bases of a phenomenological but orbital specific description of the electron-electron attraction and a realistic quantitative account of the electronic structure in the normal state. We found that a simple model which features both 'in plane' and 'out of plane' coupling with strengths $U_{\|} = 40$meV and $U_{\perp} = 48$meV respectively reproduced the experimentally observed power law behaviour of the low temperature specific heat $C_v(T)$, superfluid density $n_s(T)$ and thermal conductivity in quantitative detail. Moreover, it predicts that the quasi-particle spectrum on the γ -sheet is fully gaped and the corresponding order parameter breaks the time reversal symmetry. We have also investigated the stability of this model to inclusion of further interaction constants in particular between orbitals contributing to the γ sheet of the Fermi surface and the α and β sheets. We found that the predictions of the model are robust under such changes. Finally, we have incorporated a description of weak disorder into the model and explored some of its consequences. For example we demonstrated that the disorder has a more significant effect on the f-wave component of the order parameter than on the p-wave one.

MgB_2 How Many Gaps?

A. Gabovich

Crystal Physics Department, Institute of Physics, National Academy of Sciences, prospekt Nauki 46, MSP 03028 Kiev-28, UKRAINE

Abstract

The available experimental data on MgB_2 were revisited. It was shown that they are inconsistent with the direct application of the widely accepted theory based on the multiple-gap concept of superconductivity. An alternative approach suggesting an inhomogeneous

spatial distribution of T_c's (and gaps) was developed and it was shown that the experimental heat capacity data can be easily fitted by such quasi-random distributions. Although the approach is phenomenological, it is based on the point-contact and tunnel measurements as well as on the percolative structure of superconducting MgB_2 samples revealed by resistive studies (Korean+American+Polish collaboration).

Quantum Computing with Small superconductors

J.F. Annett, J. Walker and B.L. Gyorffy

H.H. Wills Physics Laboratory, University of Bristol, Royal fort, Tyndall Avenue, Bristol BS8 1TL, United Kingdom

Abstract

Superconductors and Superfluids have the unique property of macroscopic quantum coherence. This makes them ideal candidates to physically implement the qubits of quantum information and computation. Mesoscopic superconducting devices can be fabricated in any desired geometry using modern lithographc techniques. Recently quantum state control has been demonstrated in two types of mesoscopic superconducting device, relying on quantization of charge and flux respectively. Quantum coherent coupling between two such devices has also been achieved. We review these experiments and examine in detail the question of whether quantum entanglement of two macroscopic superconductors has been or can be achieved in these experiments.

Vortices in Josephson array insulators interacting with non-classical microwaves

A. Vourdras

Department of Computing, University of Bradford, Bradford BD7 1DP, United Kingdom

Abstract

A Josephson array insulating ring is considered where vortices circulate with a high mobility. The ring contains a weak link through which the vortices tunnel (dual Josephson junction for vortices). This devices interacts with non-classical microwaves. The time evolution of the system is calculated. The results show: 1. the exchange of energy between the device and the microwaves 2.the interplay between the quantum noise in the microwaves and the quantum noise in the vortex current 3.the entanglement between vortices and microwaves.

Effects of Random Hopping Integrals on Disordered D-Wave Superconductors

R. Moradian[1], J.F. Annett and B.L. Gyorffy

[1] *Physics Department, Faculty of Science, Razi University, Kermanshah, Iran*

[2] *H.H. Wills Physics Laboratory, University of Bristol, Royal fort, Tyndall Avenue, Bristol BS8 1TL, United Kingdom*

Abstract

We study the density of states of a single impurity in a d-wave superconductor, such as Ni in BSCCO. We show that changes of the effective hopping between the impurity and the host leads to significant changes to the impurity bound state solutions as found in the solution to the self-consistent Bogoliubov de Gennes equations. We compare these results to recent STM experiments by Davis and collaborators.

5 General Workshop/Conference Announcements

5.1 International Workshop on Ferromagnetic Semiconductors

A Safellite Meeting of the SRS User Meeting

SRS Daresbury Laboratory, Warrington, UK

11 - 12 September 2003

The workshop is now open for registration. Please visit

`http://www.srs.ac.uk/srum/satellite_1.htm`.

Programme

Thursday 11 September 2003

14:00 G. van der Laan (Daresbury) : Opening remarks
14:10 Tomas Jungwirth (Austin / Prague) : General introduction
15:10 Oliver Rader (Bessy) : Photoemission on DMS
15:40 Tea/Coffee break
16:10 Bryan Gallagher (Nottingham) : Materials development
17:10 Tomasz Story (Warsaw) : New spintronic developments
18:10 End of session
19:30 Dinner

Friday 12 September 2003

09:00 Russell Cowburn (Durham) : Magnetic nanodots special
10:00 Ulrich Hillebrecht (Karlsruhe) : XMCD on DMS
10:30 Coffee break
11:00 Hermann Durr (Bessy) : Femtosecond dynamics in MM
12:00 Thomas Schulthess (ORNL) : Electronic state of DMS
13:00 Closing remarks

Further information can be found at `http://www.srs.ac.uk/srum/satellite_1.htm` .

Gerrit van der Laan (Scientific organiser)
Sue Waller (Conference office)

5.2 11th International Conference on Intergranular and Interphase Boundaries (iib2004)

Queen's University Belfast

25th-29th July, 2004

http://www.iib2004.org

The next three-yearly international conference iib2004 will mix theorists and experimentalists in a number of topics in interface science.

Poster presentations are solicited.

Please check the website above for updates.

Mike Finnis
Conference Chair

6 General Job Announcements

PostDoc in Computational Spintronics at the Molecular Level Trinity College Dublin, Ireland

One Postdoctoral fellowship is available in the Computational Spintronics group at Trinity College Dublin. The successful candidate will be involved in one of the following computational projects, sponsored by the prestigious newly awarded Science Foundation of Ireland Investigator Award: 1) ferromagnetism in highly confined semiconductor nanostructures, 2) spin-transport in carbon based systems, 3) spin-transport in metallic nanojunctions, 4) spin-transport in large organic molecules. The specific project will be decided based on the specific interest and background of the successful candidate.

The fellowship, tenable for up to 4 years, will commence on or after the 1st October 2003 with an annual salary depending on the experience of the candidate. The Physics Department at Trinity College Dublin has a long and distinguished history of research. Currently the department is host of the prestigious first phase of Science Foundation of Ireland Nanotechnology projects, attracting world class researchers and establishing internationally competitive facilities. Finally it is worth mentioning that Dublin is a vital, young European capital, and a very pleasant place to live.

Ideally the candidate must have experience in either numerical quantum transport, or density functional theory methods. Candidates for this fellowship are invited to send a CV, a brief description of their research interests and their experience, a full publication list and the contact address of at least two referees by post or e-mail to:

Dr. Stefano Sanvito
Department of Physics
Trinity College
Dublin 2, Ireland
Tel: +353-1-6083065
Fax: +353-1-6711759
E-mail: sanvitos@tcd.ie

Information about the research activity may be found at:
http://www.tcd.ie/Physics/People/Stefano.Sanvito/ .
Further particulars regarding the Fellowship may also be obtained from Dr. Sanvito.

PhD Positions in Computational Spintronics at the Molecular Level
Trinity College Dublin, Ireland

Four PhD studentships are available in the Computational Spintronics group at Trinity College Dublin. The successful candidates will be involved in one of the following computational projects, sponsored by the prestigious newly awarded Science Foundation of Ireland Investigator Award: 1) ferromagnetism in highly confined semiconductor nanostructures, 2) spin-transport in carbon based systems, 3) spin-transport in metallic nanojunctions, 4) spin-transport in large organic molecules.

All the projects will involve the development and the numerical implementation quantum transport techniques combined with density functional or other electronic structure methods. These will be under the supervision of Dr. S. Sanvito, and will involve strong collaborations with several groups both in Europe and the USA. Visiting periods to several Institutions are planned.

The studentships will commence on the 1st October 2003 with an annual salary of 12.700 Euro. The Physics Department at Trinity College has a long and distinguished history of research. Currently the department is host of the prestigious first phase of Science Foundation of Ireland Nanotechnology projects, attracting world class researchers and establishing internationally competitive facilities. Finally it is worth mentioning that Dublin is a vital, young European capital, and a very pleasant place to live.

Candidates for these studentships are invited to send a CV including the full address of two potential referees by post or e-mail to:

Dr. Stefano Sanvito
Department of Physics
Trinity College
Dublin 2, Ireland
Tel: +353-1-6083065
Fax: +353-1-6711759
E-mail: sanvitos@tcd.ie

Information about the research activity may be found at:
http://www.tcd.ie/Physics/People/Stefano.Sanvito/ .
Further particulars regarding the Studentships may also be obtained from Dr. Sanvito.

PhD Studentship

Instituut-Lorentz for Theoretical Physics, Universiteit Leiden, The Netherlands

A PhD studentship is available at the Instituut-Lorentz for Theoretical Physics of Leiden University in the Netherlands, in the group of Dr. Claudia Filippi, starting immediately. The position is for 4 years and is expected to lead to a PhD thesis.

The project will focus on applying and further developing the quantum Monte Carlo method (one of the most accurate electronic structure approaches available) for the study of the challenging problem of the excited states of photoactive biomolecules. The focus of the project will be the theoretical investigation of the physical behavior of these systems, in particular the interplay between their microscopic structure and spectral functions.

Applications (containing contact details, CV and names of two referees) and requests for further information should be sent to filippi@lorentz.leidenuniv.nl.

Dr. Claudia Filippi

Universiteit Leiden
Instituut-Lorentz for Theoretical Physics
P.O. Box 9506
NL-2300 RA Leiden
The Netherlands

E-mail: filippi@lorentz.leidenuniv.nl

POSTDOCTORAL POSITION

Institute for Solid State Research, Research Centre Jülich, Germany

Applications are invited for a postdoctoral position at the Research Centre Jülich in the field of nanomagnetism. The position is available for 2 years from 1 October 2003 and funded by the Deutsche Forschungs- gemeinschaft (DFG) through a national Priority Programme. Extension is possible. The project is to develop computational tools and theoretical approaches for excitation spectra in magnetic materials in collaboration with Dr. Arno Schindlmayr and Prof. Stefan Blgel. In particular, it involves an implementation of the GW approximation within the all-electron FLAPW method and its application to study quasiparticle excitations and corresponding lifetimes in magnetic materials.

The Institute for Solid State Research at the Research Centre Jlich has a strong profile in the theory of nanomagnetism. Established research lines focus, for instance, on the magnetic properties of low-dimensional structures, such as surfaces, quantum wires and clusters, as well as spin-dependent transport. These activities are now extended to dynamical magnetization processes and excitations, which are responsible for the performance of magnetic switches and underlie the exciting new field of spintronics. The advertised position is part of this effort.

The position is open to applicants of all nationalities. The salary is according to the BAT IIa pay scale. A strong background in electronic- structure theory and experience in the development of complex computer programmes are desirable. Applications including a curriculum vitae, a list of publications and a summary of the relevant qualifications for this position should be addressed to

Dr. Arno Schindlmayr
Institut für Festkörperforschung
Forschungszentrum Jülich
52425 Jülich
Germany
Email: A.Schindlmayr@fz-juelich.de

DOCTORAL STUDENT POSITION (PhD)

Institute for Numerical Research in the Physics of Materials (IRRMA)

Lausanne, Switzerland

The Institute for Numerical Research in the Physics of Materials (IRRMA) at the EPFL in Lausanne is seeking an outstanding PhD student to perform research in the domain of first-principles electronic structure calculations and atomic-scale simulation

(see also `http://irrmawww.epfl.ch/~pasquarello/G3.html`).

The position, immediately available, requires a universitary degree in physics or physical chemistry (or equivalent), which should have been obtained by the starting date. The candidate will have teaching duties and shall prepare a doctoral thesis at EPFL. A good background in quantum mechanics and previous experience in FORTRAN programming are required.

The interested candidates should send as soon as possible their (1) curriculum vitae, (2) the list of passed examinations and relative marks, and (3) confidential letters of recommendation to:

Prof. Alfredo Pasquarello
ITP-SB-EPFL and IRRMA
PPH-Ecublens
CH-1015 Lausanne
Switzerland
Phone: +41 21 6934416
email: Alfredo.Pasquarello@epfl.ch

POST-DOCTORAL POSITION

Institute for Numerical Research in the Physics of Materials (IRRMA)

Lausanne, Switzerland

There is currently a post-doctoral position available for a talented and motivated individual at the Institute for Numerical Research in the Physics of Materials (IRRMA) of the EPFL in Lausanne. The position is for one year and could be extended for a second one. This individual will join research projects in computational condensed matter physics. The research domain covers topics in atomic-scale simulation

(see `http://irrmawww.epfl.ch/~pasquarello/G3.html`).

Previous experience with computational techniques based on density functional theory is requested.

The interested candidates should send their (1) curriculum vitae, (2) publication list, (3) one or two reprints representative of previous research, and (4) confidential letters of recommendation to:

Prof. Alfredo Pasquarello
ITP-SB-EPFL and IRRMA
PPH-Ecublens
CH-1015 Lausanne
Switzerland
Phone: +41 21 6934416
email: Alfredo.Pasquarello@epfl.ch

Postdoctoral/Research Associate Positions in Theory of Nanostructures

National Renewable Energy Laboratory (NREL)

`http://www.sst.nrel.gov`

NREL's Solid State Theory Group is looking to fill one Postdoctoral and one Research Associate position in the exciting area of Electronic Structure Theory of Semiconductor Nanostructures. The work involves developing new methodologies capable of describing large nanostructures as well as application of our newly developed algorithms for million atom nanostructures. The duration of the positions are up to 3 years. The salary range is $45,000 - $65,000/year, depending on qualifications and rank (postdoc vs. research associate). Applicants are expected to have a strong background in solid-state theory. The positions are with Alex Zunger, Solid State Theory Group Leader. The start date is during the fall of 2003 or early 2004. Applications for both positions are being considered now. For more details about ongoing work, see `http://www.sst.nrel.gov`.

The Solid State Theory Group currently consists of ten Ph.D.'s in condensed matter theory and interacts with a broad range of experimentalists. Furthermore, the group has outstanding computational facilities: a dedicated local computing system consisting of a 16 node SGI Origin 2000, a 44 processor Linux cluster, 4 Sun Ultra 80 workstations and remote access to IBM-SP supercomputers at NREL and NERSC, Berkeley. The group has an excellent basic-research atmosphere, and is located in the beautiful Rocky Mountains. Consult our web page for additional information on the group, its history, research subjects, publications, current and past personnel and facilities.

Interested candidates should send immediately curriculum vitae, list of publications (including preprints of unpublished papers if possible), and arrange for two to three references addressed to:

Alex Zunger, M/S 3213
Solid State Theory Group
National Renewable Energy Laboratory
1617 Cole Boulevard
Golden, Colorado 80401

Clarification or further details can be obtained via email to azunger@nrel.gov.

NREL is an equal opportunity employer and proud of its commitment to diversity. Women and minorities are encouraged to apply.

Two Post-doctoral Researchers in Computational Mineral Physics

Department of Earth Sciences, University College London, U.K.

We seek to appoint two post-doctoral scientists to work for up to 2.5 years in the Computational Mineral Physics area on a NERC funded Collaborative Consortium on "Deep Earth Systems".

The positions are to carry out work on understanding

(a) the mineralogical processes involved in core-mantle interactions, and

(b) the elastic, electronic and defect properties of lower mantle minerals, both using atomistic and quantum mechanical modelling methods.

Further information can be found at

http://www.earth.ucl.ac.uk/department/vacancies/MineralPhysics.htm

or by contacting

Dr. John Brodholt (j.brodholt@ucl.ac.uk) or Prof. David Price (d.price@ucl.ac.uk).

7 Abstracts

Neptunium octupole and hexadecapole motifs in NpO_2 directly from electric dipole (E1) enhanced x-ray Bragg diffraction

S.W. Lovesey[1], E. Balcar[2], C. Detlefs[3], G. van der Laan[4], D.S. Sivia[1] and U. Staub[5]

[1] *ISIS Facility, Rutherford Appleton Laboratory, Oxfordshire OX11 0QX, UK*

[2] *TU Vienna, Atominstitut, Stadionallee 2, A-1020 Vienna, Austria*

[3] *ESRF, BP 220, F-38043, Grenoble, France*

[4] *Daresbury Laboratory, Warrington, Cheshire WA4 4AD, UK*

[5] *Swiss Light Source, CH-5232 Villigen PSI, Switzerland*

Abstract

The phase transition in NpO_2 at $T_0 \approx 25.5$ K is accompanied by the onset of superlattice reflections in the x-ray Bragg diffraction pattern, with intensity enhanced by an electric dipole (E1) event. Additional experiments using other techniques indicate no ordering at T_0 of Np magnetic moments. Absence of long-range magnetic order below T_0 fits with the outcome of a polarization analysis of superlattice intensities at 12 K; signals are observed in both the unrotated ($\sigma'\sigma$) and rotated ($\pi'\sigma$) channels of scattering while magnetic (dipole) moments would contribute only in the rotated channel. We demonstrate that these empirical findings, together with a narrow energy profile of the Bragg intensity at the Np M_4 edge, are consistent with magnetic and charge contributions to the E1 Bragg amplitude described by Np $5f$ multipoles of ranks 3 (octupole) and 4 (hexadecapole). Key to our understanding of the x-ray diffraction data gathered in the vicinity of the Np M_4 edge is recognition of an exchange field creating $3d_{3/2}$ core-level structure. The particular importance of the exchange field at the Np M_4 edge is emphatically revealed in calculations of the corresponding x-ray absorption spectrum with and without the core-valence interaction. From the experimental information about NpO_2 we can infer a ground-state wavefunction for the Np $5f^3$ valence shell and estimate saturation values for the octupole and hexadecapole. We are led to null values for Np multipoles of ranks 2 (quadrupole) and 5 (triakontadipole).

(Published in J. Phys.: Condens. Matter **15** 4511-4518 (2003))

Reprints from: g.vanderlaan@dl.ac.uk

X-ray magnetic circular dichroism study of $SmAl_2$ using the $M_{4,5}$ X-ray absorption edges

S. S. Dhesi, P. Bencok, and N. B. Brookes
European Synchrotron Radiation Facility, F-38043 Grenoble, France
G. van der Laan
Magnetic Spectroscopy, Daresbury Laboratory, Warrington WA4 4AD, UK
R. M. Gal'/era
Laboratoire de Magnetismé Louis Néel,
Associé à l'Université Joseph Fourier de Grenoble,
Centre National de la Recherche Scientifique, Grenoble Cedex, France

Abstract

The application of x-ray magnetic circular dichroism sum rules to the $M_{4,5}$ edges of rare-earth metals has been developed for Sm^{3+}. The jj mixing of intensities between the spin-orbit split $M_{4,5}$ edges and the influence of the magnetic dipole term, $\mathbf{T}$, on the sum rules have been evaluated by comparison with results from neutron scattering and magnetometry. This analysis leads to the unusual result that $\langle T_z \rangle$ is parallel to the orbital magnetic moment, $\langle L_z \rangle$, but antiparallel to the spin magnetic moment, $\langle S_z \rangle$.

(Journal of Applied Physics **93**, 8337-8339 (2003))
Reprints from: g.vanderlaan@dl.ac.uk

Coordination Dependence of Hyperfine Fields of 5sp Impurities on Ni Surfaces

Phivos Mavropoulos
IFF, Forschingszentrum Juelich, D-52425 Juelich, Germany

Abstract

We present first-principles calculations of the magnetic hyperfine fields H of 5sp impurities on the (001), (111), and (110) surfaces of Ni. We examine the dependence of H on the coordination number by placing the impurity in the surfaces, on top of them at the adatom positions, and in the bulk. We find a strong coordination dependence of H, different and characteristic for each impurity. The behavior is explained in terms of the on-site s-p hybridization as the symmetry is reduced at the surface. Our results are in agreement with recent experimental findings.

(cond-mat/0307052)
Contact person: ph.mavropoulos@fz-juelich.de

A KKR Green function formalism for ballistic transport

Ph. Mavropoulos[(1)], N. Papanikolaou[(2)], P. H. Dederichs[(1)]
[(1)] *IFF, Forschingszentrum Juelich, D-52425 Juelich, Germany*
[(2)] *Institute of Microelectronics, NCSR "Democritos", 15310 Ag. Paraskevi, Attiki, Greece*

Abstract

We develop a method for the calculation of ballistic transport from first principles. The multiple scattering screened Korringa-Kohn-Rostoker (KKR) method is combined with a Green function formulation of the Landauer approach for the ballistic transport. We obtain an efficient O(N) algorithm for the calculation of ballistic conductance through a scattering region connected to semi-infinite crystalline leads. In particular we generalize the results of Baranger and Stone in the case of Bloch wave boundary conditions and we discuss relevant properties of the S-matrix. We consider the implications on the application of the formalism in conjunction with a cellular multiple scattering description of the electronic structure, and demonstrate the convergence properties concerning the angular momentum expansions.

(cond-mat/0306604)
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Role of the Interface Region on the Optoelectronic Properties of Silicon Nanocrystals Embedded in SiO_2

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C. Spinella, F. Iacona
CNR-IMM, Sezione di Catania, I-95121 Catania, Italy

Abstract

Light emitting silicon nanocrystals embedded in SiO_2 have been investigated by x-ray absorption measurements in total electron and photoluminescence yields, by energy filtered transmission electron microscopy and by *ab-initio* total energy calculations. Both experimental and theoretical results show that the interface between the silicon nanocrystals and the surrounding SiO_2 is not sharp: an intermediate region of amorphous nature and of variable composition links the crystalline Si with the amorphous stoichiometric SiO_2. This region plays an active role in thein the light emission process.

(Physical Review B August 2003)
Contact person: ossicini@unimo.it

Magnetic Interactions in Transition-Metal Oxides

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PRESTO, JST

Abstract

The correct understanding of the nature and dynamics of interatomic magnetic interactions in solids is fundamentally important. In addition to that it allows to address and solve many practical questions such as stability of equilibrium magnetic structures, designing of magnetic phase diagrams, the low-temperature spin dynamics, etc. The magnetic transition temperature is also related with the behavior of interatomic magnetic interactions. One of the most interesting classes of magnetic compounds, which exhibits the rich variety of the above-mentioned properties in the transition-metal oxides. There is no doubts that all these properties are related with details of the electronic structure. In the spin-density-functional theory (SDFT), underlying many modern first-principles electronic structure methods, there is a certain number of fundamental theorems, which in principles provides a solid theoretical basis for the analysis of the interatomic magnetic interactions. One of them is the magnetic force theorem, which connects the total energy change with the change of single-particle energies obtained from solution of the Kohn-Sham equations for the ground state. The basic problem is that in practical implementations SDFT is always supplemented with additional approximations, such as local-spin-density approximation (LSDA), LSDA + Hubbard U, etc., which are not always adequate for the transition-metal oxides. Therefore, there is not perfect methods, and the electronic structure we typically have to deal with is always approximate. The main purpose of this article, is to show how this, sometimes very limited information about the electronic structure extracted from the conventional calculations can be used for the solution of several practical questions, accumulated in the field of magnetism of the transition-metal oxides. This point will be illustrated for colossal-magnetoresistive manganites, double perovskites, and magnetic pyrochlores. We will review both successes and traps existing in the first-principle electronic structure calculations, and make connections with the models which capture the basic physics of the considered compounds. Particularly, we will show what kind of problems can be solved by adding the Hubbard U term on the top of the LSDA description. It is by no means a panacea from all existing problems of LSDA, and one should clearly distinguish the cases when U is indeed indispensable, play a minor role, or may even lead to the systematic error.

(To be published in "Recent Research Developments in Magnetism and Magnetic Materials", Transworld Research Network)
(cond-mat/0305668)
Contact person: igor@issp.u-tokyo.ac.jp

Electronic and positron properties of zinc-blende structure of GaN, AlN, and their alloy $Ga_{1-x}Al_xN$

Yarub Al-Douri
Department of Physics, Faculty of Science, National University of Singapore, Singapore 119260

Abstract

Electronic and positron band structures and charge densities of GaN, AlN, and their alloy $Ga_{0.5}Al_{0.5}N$ in zinc-blende structure using the empirical pseudopotential method are investigated. For the ternary alloy Ga12xAlxN, the virtual crystal approximation is coupled with the pseudopotential method. The energies along G, X, and L of Ga12xAlxN alloy as a function of the alloy concentration are calculated. Angular correlation of positron annihilation radiation along different crystallographic directions in GaN, AlN, and $Ga_{0.5}Al_{0.5}N$ is calculated. Other quantities such as ionicity character and bulk modulus by means of recent models with respect to the alloy concentration are discussed.

(JOURNAL OF APPLIED PHYSICS VOLUME 93, NUMBER 12, pp. 9730, 15 JUNE 2003)
Contact person: yaldouri@yahoo.com

Vacancy formation and O adsorption at the Al(111) surface

Adam Kiejna
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Abstract

First-principles methods are used to study the vacancy formation energy and its variation with depth, the energetics of the interaction of two point defects, adsorbed oxygen atom and vacancy, as well as substitutional oxygen adsorption at the Al(111) surface. The stability of different configurations of vacancies and oxygen atoms is examined. The vacancy formation energy decreases with the depth of the vacancy. Vacancies in subsurface layers increase the binding of oxygen adatoms in on-surface hollow sites. The surface and subsurface substitutional sites appear to be unstable for oxygen adsorption and are not stabilized by simultaneous on-surface adsorption.

(submitted to: Physical Review B)
Latex-file available from: kiejna@ifd.uni.wroc.pl

Impurity scattering and quantum confinement in giant magnetoresistance systems

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Jörg Binder
Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany
Ingrid Mertig
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Abstract

Ab initio calculations for the giant magnetoresistance (GMR) in Co/Cu multilayers are presented. The electronic structure of the multilayers and the scattering potentials of point defects therein are calculated self-consistently. Residual resistivities are obtained by solving the quasi-classical Boltzmann equation including the electronic structure of the layered system, the anisotropic scattering cross sections derived by a Green's function method and the vertex corrections. Furthermore, the influence of scattering centers at the interfaces and within the metallic layers is incorporated by averaging the scattering cross sections of different impurities at various sites. An excellent agreement of experimental and theoretical results concerning the general trend of GMR in Co/Cu systems depending on the type and the position of impurities is obtained. Due to the quantum confinement in magnetic multilayers GMR can be tailored as a function of the impurity position. In Co/Cu systems impurities in the Co layer lead to high GMR values.

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Landauer conductance of tunnel junctions: Strong impact from boundary conditions

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Abstract

We present model calculations for the Landauer conductance of tunnel junctions. The tunneling of free electrons through a rectangular potential barrier is considered. The conductance of a finite number of barriers was calculated using a transfer matrix method. The periodic arrangement of the same barriers was described by a Kronig-Penney model to calculate the band structure and from that the conductance of a point contact in the ballistic limit. The comparison of both results elucidated the importance of the boundary conditions. Caused by resonant scattering in the superlattice the conductance is overestimated by the order of 1/t, the transmission coefficient of the single barrier. In the case of metallic multilayers these interferences are of minor importance. In conclusion, the application of the Landauer formula to periodic lattices to describe the tunneling conductance of a single barrier is not correct.

(Phil. Mag., accepted)
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Field-doping of C_{60} crystals: Polarization and Stark splitting

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Abstract

We investigate the possibility of doping C_{60} crystals by applying a strong electric field. For an accurate description of a C_{60} field-effect device we introduce a multipole expansion of the field, the response of the C_{60} molecules, and the Stark splitting of the molecular levels. The relevant response coefficients and splittings are calculated *ab initio* for several high symmetry orientations. Using a group theoretic analysis we extend these results to arbitrary orientations of the C_{60} molecules with respect to the external field. We find that, surprisingly, for the highest occupied (HOMO) and the lowest unoccupied molecular orbital (LUMO), respectively, the two leading multipole components lift the degeneracy of the molecular level in the same way. Moreover the relative signs of the splittings turn out to be such that the splittings add up when the external field induces charge into the respective level. That means that when charge carriers are put into a level, its electronic structure is strongly modified. Therefore, in general, in C_{60} field-effect devices charge is not simply put into otherwise unchanged bands, so already because of this their physics should be quite different from that of the alkali-doped fullerenes.

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Spin-distribution functionals and correlation energy of the Heisenberg model

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Abstract

We analyse the ground-state energy and correlation energy of the Heisenberg model as a function of spin, both in the ferromagnetic and in the antiferromagnetic case, and in one, two and three dimensions. First, we present a comparative analysis of known expressions for the ground-state energy $E_0(S)$ of *homogeneous* Heisenberg models. In the one-dimensional antiferromagnetic case we propose an improved expression for $E_0(S)$, which takes into account Bethe-Ansatz data for $S = 1/2$. Next, we consider *inhomogeneous* Heisenberg models (e.g., exposed to spatially varying external fields). We prove a Hohenberg-Kohn-like theorem stating that in this case the ground-state energy is a functional of the spin distribution, and that this distribution encapsulates the entire physics of the system, regardless of the external fields. Building on this theorem, we then propose a local-density-type approximation that allows to utilize the results obtained for homogeneous systems also in inhomogeneous situations. We conjecture a scaling law for the dependence of the correlation functional on dimensionality, which is well satisfied by existing numerical data. Finally, we investigate the importance of the spin-correlation energy by comparing results obtained with the proposed correlation functional to ones from an uncorrelated mean-field calculation, taking as our example a linear spin-density wave state.

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Density-functional calculation of ionization energies of current-carrying atomic states

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Abstract

Current-density-functional theory is used to calculate ionization energies of current-carrying atomic states. A perturbative approximation to full current-density-functional theory is implemented for the first time, and found to be numerically feasible. Different parametrizations for the current-dependence of the density functional are critically compared. Orbital currents in open-shell atoms turn out to produce a small shift in the ionization energies. We find that modern density functionals have reached an accuracy at which the remaining difference to experiment is comparable in size to the effect of small current-related terms appearing in open-shell configurations.

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Variational calculation of many-body wave functions and energies from density-functional theory

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Abstract

A generating coordinate is introduced into the exchange-correlation functional of density-functional theory (DFT). The many-body wave function is represented as a superposition of Kohn-Sham (KS) Slater determinants arising from different values of the generating coordinate. This superposition is used to variationally calculate many-body energies and wave functions from solutions of the KS equation of DFT. The method works for ground and excited states, and does not depend on identifying the KS orbitals and energies with physical ones. Numerical application to the Helium isoelectronic series illustrates the method's viability and potential.

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A bird's-eye view of density-functional theory

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Abstract

This paper is the outgrowth of lectures the author gave at the Chemistry Institute of the University of Sao Paulo at Sao Carlos, Brazil, and at the VIII'th Summer School on Electronic Structure of the Brazilian Physical Society. It is an attempt to introduce density-functional theory (DFT) in a language accessible for students entering the field or researchers from other fields. It is not meant to be a scholarly review of DFT, but rather an informal guide to its conceptual basis and some recent developments and advances. The Hohenberg-Kohn theorem and the Kohn-Sham equations are discussed in some detail, including comparisons with the equations of Thomas-Fermi, Hartree-Fock, and Dyson. Approximate density functionals, selected aspects of applications of DFT, and a variety of extensions of standard DFT are also discussed, albeit in less detail. Throughout it is attempted to provide a balanced treatment of aspects that are relevant for chemistry and aspects relevant for physics, but with a strong bias towards conceptual foundations. The paper is intended to be read before (or in parallel with) one of the many excellent more technical reviews available in the literature.

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Residual resistivity of (Ga,Mn)As alloys from ab initio calculations

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Abstract

The residual resistivity of diluted (Ga,Mn)As magnetic semiconductors with native compensating defects (As-antisites, Mn-interstitials) is calculated from first principles using the Kubo-Greenwood linear response theory. The concentration variations of the resistivity reflect the strength of impurity scattering and the number of carriers. In agreement with a recent experiment, the calculated resistivities are strongly correlated with the alloy Curie temperatures evaluated in terms of a classical Heisenberg Hamiltonian.

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Tight-binding study of the influence of the strain on the electronic properties of InAs/GaAs quantum dots

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Abstract

We present an atomistic investigation of the influence of strain on the electronic properties of quantum dots (QD's) within the empirical sp^3s^* tight-binding (ETB) model with interactions up to 2nd nearest neighbors and spin-orbit coupling. Results for the model system of capped pyramid-shaped InAs QD's in GaAs, with supercells containing $\sim 10^5$ atoms are presented and compared with previous empirical pseudopotential results. The good agreement shows that ETB is a reliable alternative for an atomistic treatment. The strain is incorporated through the atomistic valence force field model. The ETB treatment allows for the effects of bond length and bond angle deviations from the ideal InAs and GaAs zincblende structure to be selectively removed from the electronic-structure calculation, giving quantitative information on the importance of strain effects on the bound state energies. Effects of dot-dot coupling have also been examined to determine the relative weight of both strain field and wave function overlap.

(submitted to Phys. Rev. B)

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Nanostructures at Surfaces from Substrate-Mediated Interactions

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Abstract

Recent theoretical and experimental studies indicate that adsorbate-adsorbate interactions mediated by a solid surface can be significant enough to influence the formation of nanostructures during thin-film epitaxy. Here, we show that these electronic interactions lead to the formation of repulsive barriers surrounding small adsorbate islands at surfaces. The dependence of these barriers on island size and shape actuates sharp island-size distributions, which can be manipulated by changing growth conditions to yield selected island sizes and shapes. The existence of these interactions opens new prospects for engineering nanostructures at surfaces.

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Universal alignment of hydrogen levels in semiconductors, insulators and solutions

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Abstract

Hydrogen strongly affects the electronic and structural properties of many materials. It can bind to defects or to other impurities, often eliminating their electrical activity: this effect of defect passivation is crucial to the performance of many photovoltaic and electronic devices. A fuller understanding of hydrogen in solids is required to support development of improved hydrogen-storage systems, proton-exchange membranes for fuel cells, and high-permittivity dielectrics for integrated circuits. In chemistry and in biological systems, there have also been many efforts to correlate proton affinity and deprotonation with host properties. Here we report a systematic theoretical study (based on ab initio methods) of hydrogen in a wide range of hosts, which reveals the existence of a universal alignment for the electronic transition level of hydrogen in semiconductors, insulators and even aqueous solutions. This alignment allows the prediction of the electrical activity of hydrogen in any host material once some basic information about the band structure of that host is known. We present a physical explanation that connects the behaviour of hydrogen to the line-up of electronic band structures at heterojunctions.

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First-principles Calculations of $PuO_{2\pm x}$

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Abstract

The electronic structure of $PuO_{2\pm x}$ was studied using first-principles quantum mechanics, realized with the self-interaction corrected local spin density method. In the stoichiometric PuO_2 compound, Pu occurs in the Pu(IV) oxidation state, corresponding to a localized f^4 shell. If oxygen is introduced onto the octahedral interstitial site, the nearby Pu atoms turn into Pu(V) (f^3) by transferring electrons to the oxygen. Oxygen vacancies cause Pu(III) (f^5) to form by taking up electrons released by oxygen. At $T = 0$ the PuO_2 compound is stable with respect to free oxygen, but the delicate energy balance suggests the possible deterioration of the material during long-term storage.

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8 SCIENTIFIC HIGHLIGHT OF THE MONTH

Strength, magnetism and stability of metals and intermetallics at extreme loading conditions

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Abstract

Theoretical strength, magnetism, stability, and phase transformations in iron and the intermetallic compound Ni_3Al are studied via first-principles electronic structure calculations. Total energies are calculated as functions of parameters characterizing the tetragonal and trigonal transformation paths at various atomic volumes using the spin-polarized full-potential linearized augmented plane waves (FLAPW) method with the generalized-gradient approximation (GGA) for the exchange-correlation energy. The results are displayed in terms of contour plots of the dependence of the energy on parameters of the tetragonal or trigonal deformation and volume. Borders between various magnetic phases are shown. Whereas during tetragonal deformation, iron transforms to antiferromagnetic states, it mostly keeps its ferromagnetic ordering during trigonal deformation. The total energy difference between non-magnetic and ferromagnetic Ni_3Al in the $L1_2$ structure is very small, about 21 meV/formula unit and, therefore, magnetism does not play an important role in stabilization of the $L1_2$ structure. For iron, we discuss the results of simulated tensile tests for uniaxial loading along the [001] and [111] directions as well as for isotropic triaxial tension and compare corresponding tensile strengths. Marked anisotropy of theoretical tensile strength in [001] and [111] direction is elucidated in terms of the presence of higher-symmetry structures along the deformation paths. A table summarizing the values of theoretical tensile strengths calculated up to now is presented.

1. Introduction

The strength of materials is usually controlled by nucleation and motion of dislocations or microcracks. If such defects were not present, the material loaded in tension would only fail if the theoretical, or ideal tensile strength were reached. The stress at which this is achieved is comparable with the Young modulus of the material and it is an upper limit of stresses attainable prior to failure. Until recently loads of this magnitude were approached in studies of the mechanical behaviour of whiskers of very pure metals and semiconductors [1–5]. However, the ideal strength appears to control both the onset of fracture and dislocation nucleation in defect-free thin films and, in particular, in nano-structured materials that are currently being developed. This has been confirmed most eloquently by nanoindentation experiments (see e. g. [6–10]) which suggest that the onset of yielding at the nanoscale is controlled by homogeneous nucleation of dislocations in the small volume under the nanoindenter where stresses approach the theoretical strength. This volume is practically always dislocation free since in well-annealed samples the average dislocation spacing is about 1 μm, while the contact area as well as the depth in which large stresses are attained are of the order of 100 nm.

Theoretically, the ideal strength was studied in the past using semiempirical approaches when describing atomic interactions (for a review see e.g. [11] and the references therein; ideal shear strengths calculated for all basic cubic structures may be found in [12]). However, within such schemes parameters characterizing interatomic forces are fitted to equilibrium properties of the material studied and their transferability to the state when this material is loaded close to its theoretical strength is not warranted. In contrast, ab initio electronic structure (ES) calculations can be performed reliably for variously strained structures and are thus capable to determine the ideal strength of materials without resort to doubtful extrapolations. Nevertheless, most of the ES calculations were directed towards finding the equilibrium state of a given material that corresponds to the minimum of the total energy or towards analysis of relatively small deviations from that state. On the other hand, theoretical strength is related to the maximum force that may be applied to the material without perturbing its stability. It is usually connected with an inflexion point on the dependence of the total energy on deformation parameters.

The first paper dealing with the ideal tensile strength from the first principles was probably that of Esposito et al. [13]. However, those authors have not performed relaxations of dimensions of the loaded crystal in the directions perpendicular to the loading axis. Paxton et al. [14] and Xu and Moriarty [15] calculated shear strength for unrelaxed shear deformation. Other ab initio calculations of properties of the systems far from equilibrium have also been made, such as exploration of the structural stability, but the results were not employed to evaluate the strength [16–20].

Probably the first ab initio simulation of a tensile test, including the relaxation in perpendicular directions to the loading axis, was performed by Price et al. [21] for uniaxial loading along the [001] axis in TiC. Later, our group at the Institute of Physics of Materials in Brno initiated systematic ab initio studies of theoretical strength and stability in metals and intermetallics under extreme loading conditions. In [22], we obtained the theoretical tensile strengths for [001] and [111] loading directions in tungsten. The results compared very well with experiments performed on tungsten whiskers by Mikhailovskii et al. [23]. Further, we calculated ideal tensile strength

in NiAl [24, 25] and Cu [25]. These results found a very good response in the international solid state physics and materials science communities and established a basis for further calculations of ideal tensile strength. Li and Wang [26] computed the ideal tensile strength in Al. Kitagawa and Ogata [27, 28] studied the tensile strength of Al and AlN, but have not included Poisson contraction. The group at the University of California at Berkeley calculated ideal shear strength in Al and Cu [29, 30] as well as in W [31, 32], performed a thorough theoretical analysis of the problem of strength and elastic stability [33] and, among others, verified our values of ideal tensile strength for tungsten [32].

Further calculations of theoretical tensile strength were performed for β-SiC [34], diamond [35, 36], Si and Ge [36], Mo and Nb [37], and for Si_3N_4 [38-40]. Ideal shear strength was recently calculated for TiC, TiN and HfC [41], Si [42] and newly for Al and Cu [43]. Some calculations have been done for nanowires (amorphous Si [44], MoSe nanowires [45]), grain boundaries [46, 47], and interfaces [48].

From 1997, ab initio calculations of theoretical strength under isotropic triaxial (hydrostatic) tension (i.e., negative hydrostatic pressure) also appeared [49–54]. As the symmetry of the structure does not change during this deformation, simpler ab initio approaches may be applied.

Very recently, we have simulated a tensile test in prospective high-temperature materials, namely in transition metal disilicides $MoSi_2$ and WSi_2 with the $C11_b$ structure. This study included calculation of the tensile strength for [001] loading and analysis of bonds and their changes during the test [55, 56]. Theoretical tensile strength of iron in the loading direction [001] was determined in Refs. [57] and [58]; in [59], we compared those results to each other and calculated the tensile strength of iron for uniaxial loading in the [111] direction. Tables summarizing ab initio values of theoretical tensile strengths for various materials are given in Refs. [59-62] and, most up-to date, in Table 1 in Section 6 of the present work. Ref. [61] includes also ab initio values of shear strengths and some semiempirical results. An extensive review of the semiempirical and ab initio calculated values of uniaxial and isotropic triaxial tensile strengths as well as of shear strengths calculated up to 1999 can be found in Ref. [63].

There are more general problems of stability of materials and of phase transformations that are closely related to the tensile tests described above. Namely, the tensile test may be considered as a special case of the so-called displacive phase transformation path [16, 18]. These paths are well known in studies of martensitic transformations. Such transformations play a major role in the theory of phase transitions. They proceed by means of cooperative displacements of atoms away from their lattice sites that alter crystal symmetry without changing the atomic order or composition. A microscopic understanding of the mechanisms of these transformations is vital since they occur prominently in many materials.

Displacive phase transformations are also of interest in studies of epitaxial thin films. Pseudomorphic epitaxy of a cubic or tetragonal (001) film typically results in a strained tetragonal structure. In this case, there is a stress in the (001) plane keeping the structure of the film and of the substrate coherent, and the stress perpendicular to this plane vanishes. A tetragonal phase arises that may be stable or metastable [20]. Similarly, an epitaxial film grown on the (111) plane of a cubic substrate exhibits a trigonal deformation of its lattice, which may be considered as a uniaxial deformation along the [111] axis. In this context it is interesting to

consider the trigonal deformation path, which comprises the bcc, fcc and simple cubic structures as special cases [64-66, 18]. We have also proposed the bcc to hcp transformation path, which we investigated in iron [67] and in intermetallic compounds TiAl and NiAl [68]. Very recently, we have studied the tetragonal bcc-fcc transformation path in iron and have shown how these results may be used to predict the lattice constants and magnetic order of iron overlayers on various metallic substrates [69, 70]. This research is closely connected with the studies of iron stability performed in Refs. [71-76].

Another area of importance of the local stability of non-equilibrium phases and phase transformation paths is the structure of extended defects in solids. It was found in recent studies that atomic configurations in grain boundary (GB) regions, or at other interfaces, may contain certain metastable structures, different from the ground-state structures. For example, the 9R (α-Sm) structure was theoretically predicted and verified by high-resolution electron microscopy (HREM) at GBs in silver and copper [77, 78]. Similarly, the bcc structure was found at certain grain boundaries in copper [79]. We have shown [80] that the bcc Cu at grain boundaries is stabilized by external constraints exerted by the surrounding fcc grains and studied stabilization of higher-energy phases in pseudomorphic films [81].

Occurrence of such phases at interfaces is even more likely in more complex non-cubic alloys. For example, new structural features of TiAl, which crystallizes in tetragonal $L1_0$ structure, have been discovered recently. Abe et al. [82] found a B19-type hcp-based structure in a Ti-48at.%Al alloy quenched from the disordered phase, and Banerjee et al. [83] observed a series of structural transitions in the form of changes in the stacking sequence of the close-packed atomic planes in the Ti and Al layers in Ti/Al multilayered thin films.

Consequently, in order to explore adequately extended defects both in pure metals and alloys, in particular in intermetallics, detailed information about possible metastable structures, as well as lattice transformations connecting them, is needed. Armed with this knowledge one can predict whether an interface may be associated with a metastable structure and assess thus its stability and ability to transform to other structures (for example during deformation or due to changes in stoichiometry).

The purpose of the present paper, which is based on a recent presentation [62], is to study lattice configurations found in the course of tetragonal and trigonal displacive transformation (deformation) paths. These configurations are produced by large homogeneous distortions that transform the initial (ground-state) structure into new (higher-energy) structures with different symmetries. Such investigations are closely linked with theoretical strength and phase transformations and constitute a basis for future analyses of various configurations of extended defects in metallic materials. As specific examples, we study iron and the intermetallic compound Ni_3Al. Iron exists in both bcc and fcc modifications and has many magnetic phases, especially in thin films. Notably, fcc iron films exhibit a large variety of structural and magnetic properties that depend delicately on the thickness of the iron layer and preparation conditions [84]. Ni_3Al is the most important strengthening constituent of commercial nickel-based superalloys used extensively as structural materials for elevated temperatures applications. This phase is responsible for the high-temperature strength and creep resistance of the superalloys. Ni_3Al and a number of other intermetallic compounds with the $L1_2$ structure exhibit so-called anomalous yield behav-

ior, when their yield strength increases rather than decreases with increasing temperature. This behavior is not the result of a change in long-range order with temperature since the (Bragg) long-range parameter, S, is almost constant in Ni_3Al up to 1000 ^oC. There is now near-universal agreement that the anomaly results from the special properties of screw dislocation cores and the anisotropy in antiphase boundary energies; a review and comparison of various models are presented in Ref. [85]. Single crystals of Ni_3Al are ductile, but pure polycrystalline Ni_3Al is very brittle at room temperature because of intergranular fracture. Both iron and Ni_3Al exhibit magnetic ordering; therefore, we also study the changes of the magnetic state of these materials during deformation.

2. Displacive phase transformation paths

We consider two simple transformation paths connecting cubic structures. They are the bcc-fcc transformation path via tetragonal deformation corresponding to extension along the [001] axis (the usual Bain's path) and the trigonal deformation path that corresponds to uniaxial deformation along the [111] axis (Figs. 1 and 2).

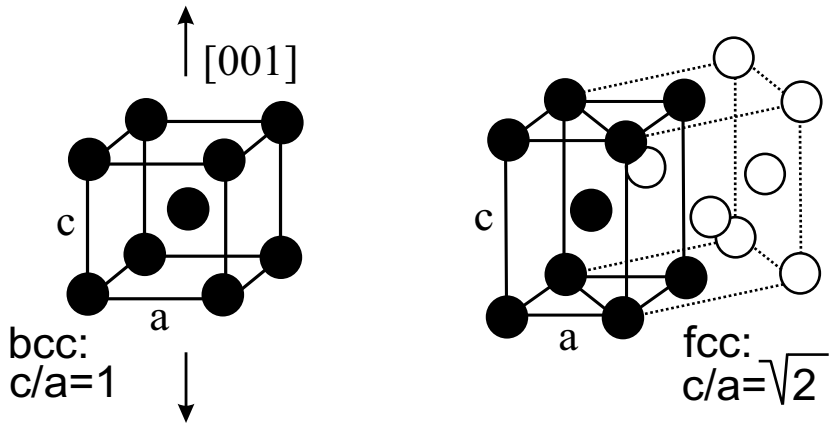

Figure 1: High-symmetry structures obtained along the tetragonal deformation path. The c and a are the length scales along the [001] and [100] directions, respectively. The original bcc cell is indicated by full circles and heavy solid lines.

In the case of tetragonal deformation path, we start with the bcc structure considered as a tetragonal one with the ratio $c/a = 1$, where c is measured along the [001] direction and a along a [100] direction. When c/a is varied, we arrive at body-centered tetragonal structures. There is one exception: for $c/a = \sqrt{2}$ the structure becomes fcc (Fig. 1).

Similarly, we may consider the bcc structure as trigonal with the ratio of $c/a = 1$, where c is measured along the [111] direction and a along a direction perpendicular to [111]. If $c/a \neq 1$, the structure becomes trigonal except for $c/a = 2$, when we attain the simple cubic (sc) structure, and $c/a = 4$, which again corresponds to the fcc structure (see Fig. 2).

When studying the behavior of the total energy along the deformation paths, one usually assumes that the atomic volume is constant. Then both deformation paths discussed above may be fully parameterized by the ratio c/a.

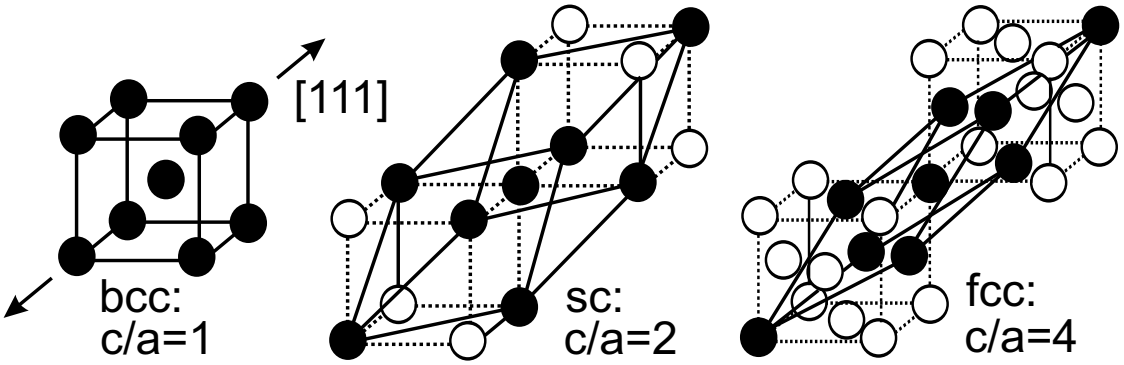

Figure 2: High-symmetry structures obtained along the trigonal deformation path. The c and a are the length scales along the [111] direction and along a direction perpendicular to [111], respectively.

Analogous deformation paths may be devised for intermetallic compounds with B2, $L1_2$ or $D0_3$ structures [18, 86]. In the $L1_2$ (Cu_3Au) structure, the atoms are at the fcc positions with the (002) planes occupied alternatively by Cu atoms and by Cu and Au atoms in the same ratio. We may consider this structure as tetragonal or trigonal with the ratio $c/a = 1$. Now, performing a tetragonal deformation, the cubic symmetry of the $L1_2$ configuration is lost and becomes tetragonal, even for $c/a = \sqrt{2}/2$, when atoms are at the bcc-like positions, but because we have two kinds of atoms, the structure does not attain the cubic symmetry. When we perform the trigonal deformation, the structure becomes trigonal except for the case of $c/a = 0.5$, when we encounter a simple-cubic-based structure that, indeed, has a cubic symmetry. For $c/a = 0.25$, the atoms adopt the bcc-like positions, but the symmetry of the structure remains trigonal. All these structures will be characterized in more details in a subsequent publication [86]. (Note different "normalization" of the ratio c/a for the $L1_2$ structure. Here we ascribed the value of $c/a = 1$ to the fcc-based configuration. Consequently, as it may be seen from Figs. 1 and 2, the bcc-based configuration, obtained by the tetragonal deformation, corresponds to $c/a = \sqrt{2}/2$, and the sc- and bcc-based structures, obtained by the trigonal deformation, correspond to $c/a = 0.5$ and $c/a = 0.25$, respectively.)

Craievich et al. [16] have shown that some energy extrema on constant-volume transformation paths are dictated by the symmetry. Namely, most of the structures encountered along the transformation paths between some higher-symmetry structures, say between bcc and fcc at the Bain's path, have a symmetry that is lower than cubic. At those points of the transformation path where the symmetry of the structure is higher, the derivative of the total energy with respect to the parameter describing the path must be zero. These are the so-called symmetry-dictated extrema. However, other extrema may occur that are not dictated by the symmetry and reflect properties of the specific material. The same is true for the transformation paths corresponding to uniaxial loading [20, 87]. Configurations corresponding to energy minima at the transformation paths represent stable or metastable structures and may mimic atomic arrangements that could be encountered when investigating thin films [20] and extended defects such as interfaces or dislocations [18, 68]. For iron and Ni_3Al, we will discuss these configurations below.

3. Tensile test simulation

To simulate a uniaxial tensile test, we start by determining the structure and total energy of the material in the ground state. Then, in the second step, we apply an elongation along the loading axis by a fixed amount ε that is equivalent to application of a certain tensile stress σ. For each value of ε, we minimize the total energy by relaxing the stresses $\sigma_{\perp 1}$ and $\sigma_{\perp 2}$ in the directions perpendicular to the loading axis. The stress σ is given by [88]

$$\sigma = \frac{c}{V}\frac{\partial E}{\partial c} = \frac{1}{Ac_0}\frac{\partial E}{\partial \varepsilon}, \tag{1}$$

where E is the total energy per repeat cell, V is the volume of the repeat cell, c is the dimension of the repeat cell in the direction of loading, A (equal to V/c ratio) is the area of the basis of the repeat cell in the plane perpendicular to the loading axis, and c_0 is the value of c in the undeformed state.

We are also interested in tensile strength at isotropic triaxial (hydrostatic) tension. In this case, we start again with the material in its ground-state structure, but the dimension of the crystal is gradually increased homogeneously in all directions. The hydrostatic stress σ is then calculated using the formula $\sigma = dE/dV$.

The inflexion point in the dependence of the total energy on elongation yields the maximum of the tensile stress; if any other instability (violation of some stability condition, soft phonon modes, magnetic spin arrangement etc.) does not occur prior to reaching the inflexion point, it also corresponds to the theoretical tensile strength, σ_{th}.

4. Methods of calculation

The atomic configurations corresponding to the deformed structures have usually a lower symmetry and, at the strength limit, they are very far from the ground state. Therefore, to get reliable structural energy differences, we must use a full-potential method for the calculations. Here we use the full-potential linearized augmented plane wave (FLAPW) code WIEN97 described in detail in Ref. [89]. The exchange-correlation energy is evaluated within the generalized-gradient approximation (GGA) [90]. This is important especially for iron, since the local density approximation does not render the ground state of iron correctly. The muffin-tin radius of iron atoms of 1.90 au is kept constant for all calculations. The number of $\boldsymbol{k}$-points in the whole Brillouin zone is equal to 6000 and the product of the muffin-tin radius and the maximum reciprocal space vector, $R_{MT}\ k_{max}$, is set to 10. The maximum l value for the waves inside the atomic spheres, l_{max}, and the largest reciprocal vector in the charge Fourier expansion, G_{max}, is equal to 12 and 15, respectively. In the case of Ni_3Al, the muffin-tin radii of both Ni and Al atoms are equal to 2.0 au, number of $\boldsymbol{k}$-points in the whole Brillouin zone is 4000, and the product $R_{MT}\ k_{max} = 8$. The values of l_{max} and G_{max} are 12 and 10, respectively.

5. Results and discussion

5.1. Iron

5.1.1. Total energies and magnetic states of tetragonally and trigonally deformed iron. We have calculated the total energy and magnetic moment of iron deformed along the tetragonal and trigonal paths at constant atomic volumes ranging from $V/V_{exp} = 0.84$ to $V/V_{exp} = 1.05$, where V_{exp} is the experimental equilibrium atomic volume of the ferromagnetic bcc iron corresponding to the lattice constant $a_{bcc} = 5.408$ au. As shown in Figs. 3 and 4, we include non-magnetic (NM), ferromagnetic (FM) and two antiferromagnetic states, namely the single-layer antiferromagnetic state (AFM1), in which the (001) or (111) planes have alternating magnetic moments ($\uparrow\downarrow\uparrow\downarrow\ldots$), and the double-layer antiferromagnetic state (AFMD), where the pairs of (001) or (111) planes have alternating magnetic moments ($\uparrow\uparrow\downarrow\downarrow\ldots$). The total energy of iron is plotted as a function of volume and the c/a ratio in Figs. 5 and 6. We show only those states the energies of which are the lowest for a given configuration. In Fig. 5, we can clearly see the "horseshoes" dividing the plane into the AFM1, AFMD and FM regions whereas the area of Fig. 6 is dominated by the FM states. The global minimum of energy is in the FM region at $c/a = 1$, $V/V_{exp} = 0.985$, which corresponds to the bcc structure. The calculated equilibrium volume is about 1.5 % lower than the experimental value, which may be considered as a very good agreement.

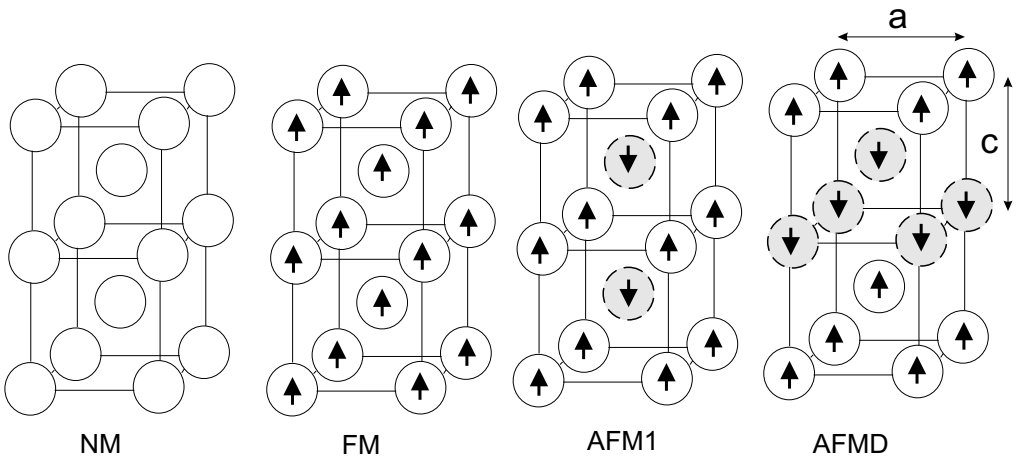

Figure 3: Non-magnetic (NM), ferromagnetic (FM), antiferromagnetic single-layer (AFM1) and antiferromagnetic double layer (AFMD) states of iron included in calculations of total energy profiles along tetragonal deformation paths.

The ground-state energy minimum is dictated by the symmetry. Any energy profile at the constant volume, obtained from Figs. 5 and 6, also exhibits the minimum at $c/a = 1$.

Let us discuss the tetragonal case first (Fig. 5). Apart from the large FM area, there are AFMD and AFM1 regions in the neighborhood of the fcc structure, which corresponds to the line $c/a = \sqrt{2}$. Note that the lattice symmetry of the fcc iron with the AFM1 and AFMD spin ordering is tetragonal and, therefore, we do not find any extremum of the total energy of these states (dictated by symmetry) at $c/a = \sqrt{2}$. In accordance with Ref. [72], we found that the fcc iron with the AFM1 or AFMD spin ordering is unstable with respect to the tetragonal deformation.

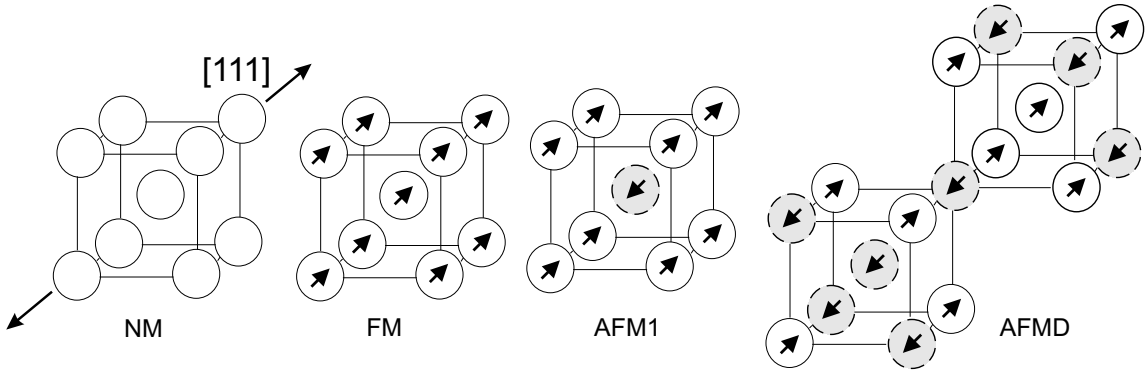

Figure 4: Non-magnetic (NM), ferromagnetic (FM), antiferromagnetic single-layer (AFM1) and antiferromagnetic double layer (AFMD) states of iron included in calculations of total energy profiles along trigonal deformation paths. (Note that these figures do not display all the (111) planes in the lattices shown).

A more detailed discussion of the tetragonal case is presented in Refs. [69, 70]. In those papers, we also showed how the contour plot presented in Fig. 5 may be used to predict the lattice parameters and magnetic states of iron overlayers at (001) substrates.

The AFMD structure with the tetragonal symmetry may be considered as a close approximation of the spin-spiral state with $\mathbf{q} = (2\pi/a)$ (0, 0, 0.6), found as the ground state of the fcc iron [91]. It will be the topic of future studies to ascertain how the non-collinearity of magnetic moments changes the borders between various magnetic phases in the (c/a, V/V_{exp}) plane. We surmise that the region of non-collinear magnetism will not be too different from the AFMD region shown in Fig. 5.

The AFM1 and AFMD states with the trigonal symmetry (Fig. 4) have mostly higher energy than the FM states and, consequently, they are nearly invisible in Fig. 6, except for the lower right corner. However, two regions of the FM states may be found in Fig. 6: FM(HS), the high-spin states (with magnetic moment higher than about 2 μ_B) and FM(LS), the low-spin states (with magnetic moment lower than about 1.2 μ_B). There is a sharp discontinuity in the magnetic moment at the border FM(HS)/FM(LS). Nonetheless, the total energy remains surprisingly smooth. The triangles in Fig. 6 denote local energy minima of fcc FM states and the square marks the point where the volume dependencies of the total energies of the fcc FM(HS) and FM(LS) states, displayed in Fig. 7, intersect. From Fig. 7 we see that the square represents a "sharp" saddle point in Fig. 6.

All total energy profiles at a constant volume $V > 0.955\ V_{exp}$ exhibit three symmetry-dictated extrema: a minimum at $c/a = 1$ (bcc structure), a maximum at $c/a = 2$ (sc structure) and a minimum at $c/a = 4$ (fcc structure). The reason is that both FM and NM structures exhibit a higher (cubic) symmetry at those values of c/a. The profile of the total energy at the constant volume $V = V_{exp}$, obtained from Fig. 6, is shown in Fig. 8. It is qualitatively similar to the total energy profiles of trigonally deformed Ta [92, 93] or Ir [18] and Cu [80] (the ground-state structure of Ir and Cu is fcc and, therefore the fcc minimum for those metals is lower than the bcc minimum).

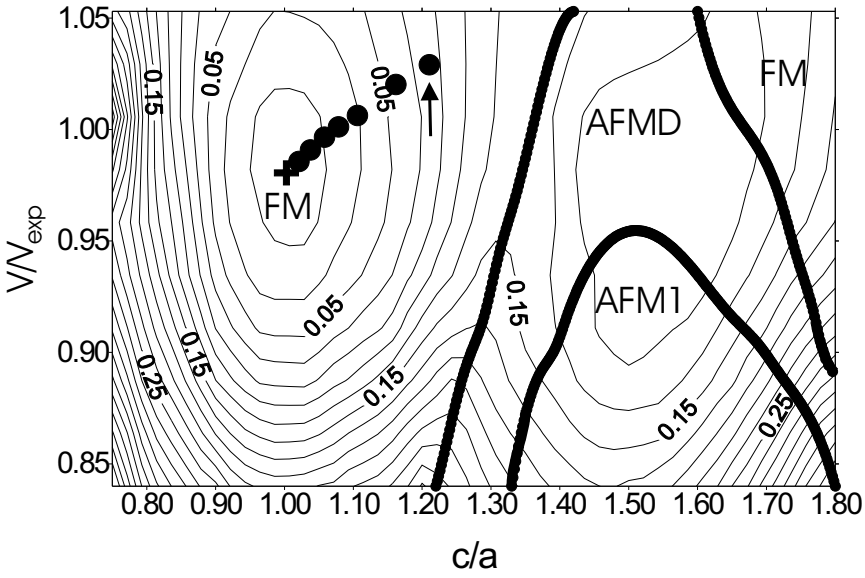

Figure 5: Total energy (per atom) of iron as a function of the tetragonal c/a ratio and volume relative to the energy of the FM bcc equilibrium state calculated within the GGA. Only states with the minimum energy are shown. The contour interval is equal to 20 meV. Thick lines show the FM/AFMD and AFMD/AFM1 phase boundaries. The cross corresponds to the global, symmetry-dictated minimum (ground state). The path representing the simulation of the tensile test for loading along the [001] direction is denoted by full circles; the highest circle marked by an arrow corresponds to the maximum stress obtained in the simulation of the tensile test.

5.1.2. Uniaxial and isotropic triaxial tensile tests. In accordance with methodology described in Sec. 3, we performed the simulation of a tensile test in iron for uniaxial loading along the [001] and [111] directions, respectively, as well as for isotropic triaxial loading corresponding to the negative hydrostatic pressure. The corresponding total energies as functions of relative elongation ε are displayed in Fig. 9(a). In case of the isotropic triaxial loading, ε corresponds to a relative extension of the bcc lattice parameter

It is seen from Fig. 9(a) that the total energy profiles have a parabolic, convex character in the neighborhood of the ferromagnetic (FM), symmetry-dictated, minimum that corresponds to the bcc structure (ground state). With increasing value of ε the curves reach (due to non-linear effects) their inflexion points (marked by vertical lines in Fig. 9(a)) and become concave. The inflexion point for [001] uniaxial loading occurs (most likely incidentally) for nearly the same elongation of $\varepsilon = 0.15$ as for the isotropic triaxial loading. In the case of the [001] tensile test, this elongation corresponds to the lattice parameter in the direction of loading equal to 6.20 au (accompanied by relaxation in [100] and [010] directions in which the lattice constant decreases to 5.12 au) and, in the case of isotropic triaxial strain, to the bcc structure with the lattice constant of 6.20 au.

The tensile stresses calculated according to formulas given in Sec. 3 are shown in Fig. 9(b). The inflexion points on the total energy profiles correspond to maximum stresses which the material may accommodate if its structure type does not change during the deformation. They are equal to $\sigma_{max}^{[001]} = 12.7$ GPa (this value was reported in our previous work [57] and is not very different

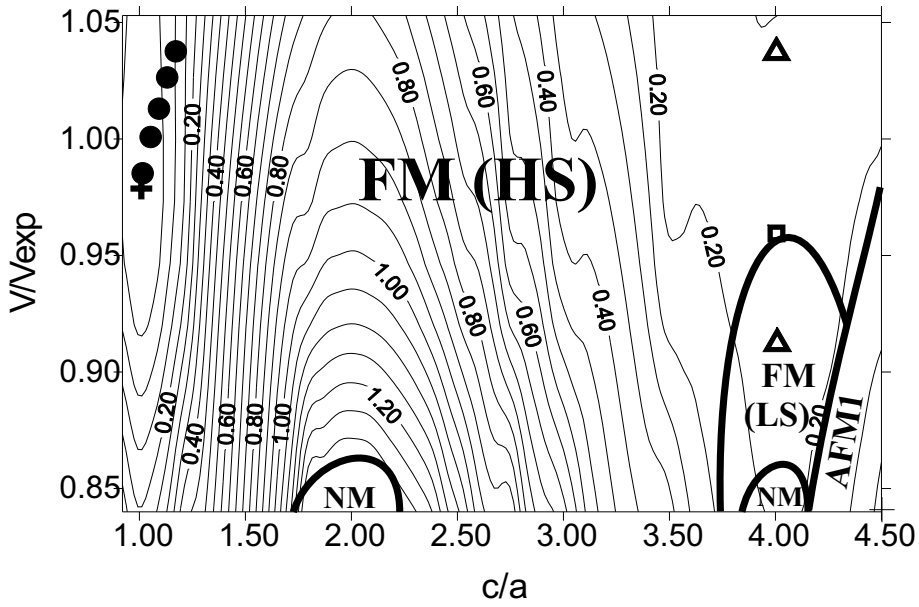

Figure 6: Total energy (per atom) of iron as a function of the trigonal c/a ratio and volume relative to the energy of the FM bcc equilibrium state, calculated within the GGA. Only states with the minimum energy are shown. The contour interval is equal to 50 meV. Thick lines show the FM(HS)/NM, FM(HS)/FM(LS), FM(LS)/NM and FM(LS)/AFM1 phase boundaries. The cross corresponds to the global symmetry-dictated minimum (ground state), the triangles show the local minima of the total energy of the fcc states in the FM(HS) and FM(LS) region at $V/V_{exp} = 1.037$ and 0.911, respectively. The square at $V/V_{exp} = 0.955$ denotes the crossing point of the dependencies of the total energy of the FM(HS) and FM(LS) fcc states on volume, presented in Fig. 7. As Fig. 7 shows, this square represents a "sharp" saddle point. The path representing simulation of the tensile test for loading along the [111] direction is denoted by full circles; the state corresponding to the maximum stress attained in the tensile test simulation ($V/V_{exp} = 1.114$, $c/a = 1.356$) lies outside the area of the figure.

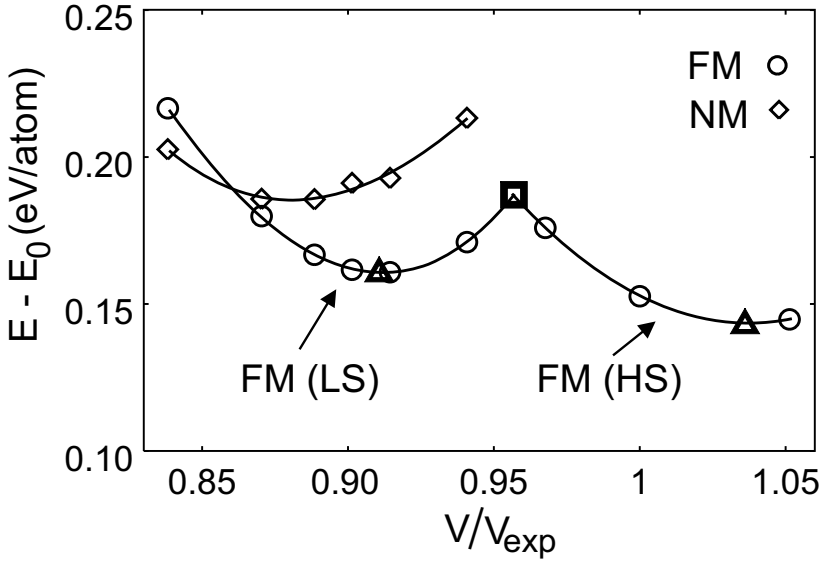

Figure 7: Total energies of the fcc FM and NM states of iron as functions of volume relative to the total energy of the FM bcc ground state. The triangles denote local energy minima (for their exact position see the description of Fig. 6), and the square corresponds to the intersection of the FM(HS) and FM(LS) curves.

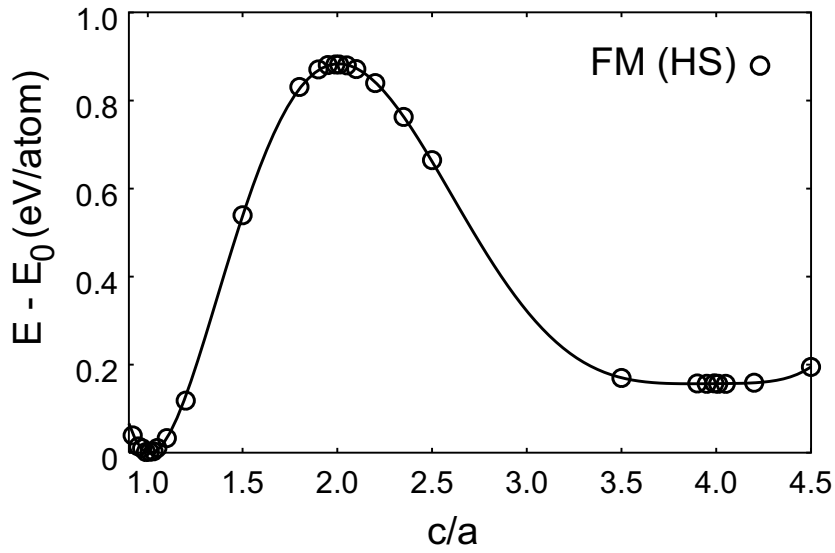

Figure 8: The profile of the total energy of trigonally deformed iron at $V/V_{exp} = 1$ (cf. with Fig. 6). All energy extrema (at $c/a = 1$, 2 and 4) are dictated by symmetry.

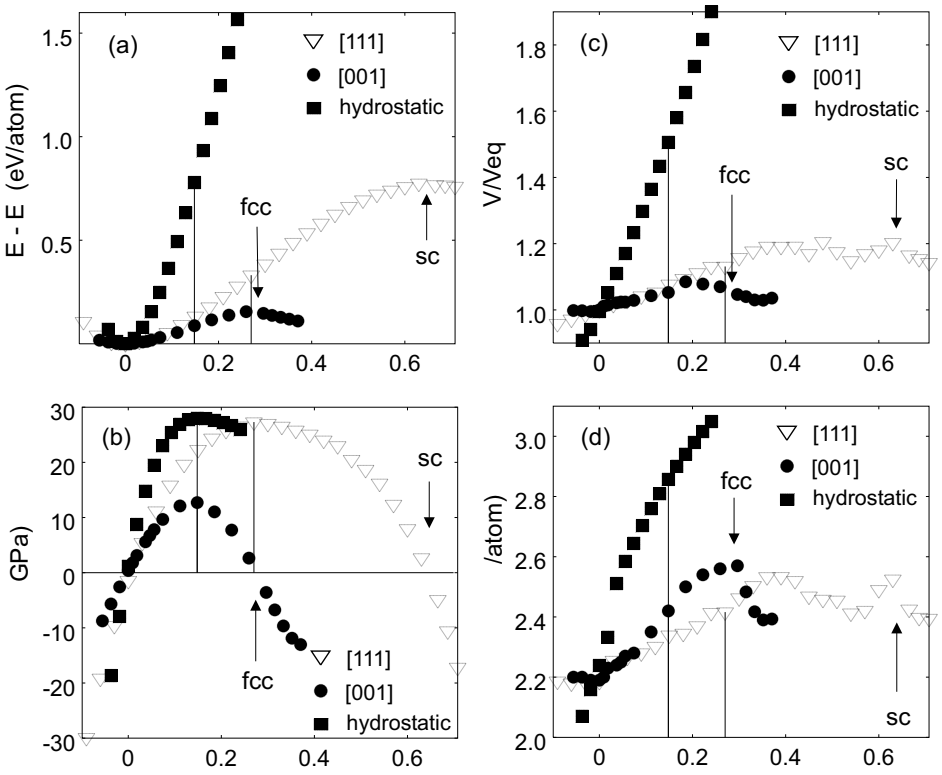

Figure 9: Total energy per atom measured with respect to the energy of the equilibrium state (a), stress (b), relative atomic volume ratio measured with respect to the equilibrium volume V_{eq} (c), and magnetic moment per atom μ (d) of FM iron loaded hydrostatically (full squares) and uniaxially along the [001] (full circles) and [111] (empty triangles) directions vs. elongation ε. The relative elongation ε reflects the changes of the lattice parameter a_{bcc} for isotropic triaxial loading and, in the case of uniaxial tensile tests, the increase/decrease of the crystal dimension in the directions of loading. The thin vertical lines mark the states exhibiting maximum stress (i.e. theoretical tensile strength). Incidentally, the maximum stresses for [001] uniaxial and isotropic triaxial (hydrostatic) loading are reached at nearly the same strain ε and, therefore, the corresponding vertical lines coincide.

from 14.2 GPa found in Ref. [58]), $\sigma_{max}^{[111]} = 27.3$ GPa and $\sigma_{max}^{[hydrostatic]} = 27.9$ GPa for uniaxial tensile test along the [001] and [111] direction and for isotropic triaxial (hydrostatic) loading, respectively. These values represent the theoretical tensile strengths provided other instabilities (soft phonon modes, etc.) do not come forth before reaching the inflexion point. In the case of iron with its large variety of magnetic phases, another instability may originate from transitions between those phases. However, as it is seen from Figs. 5 and 6, no such transition appears during tensile tests along [001] and [111] directions (all states involved up to the maximum stress lie in the FM region). A similar situation arises for isotropic triaxial deformation [54]. Other conditions of stability [88, 94] will be analyzed in a subsequent publication, but our preliminary calculations indicate that they will not be violated. It should be noted that the theoretical strength for loading in the [111] direction, equal to 27.3 GPa, is nearly the same as that obtained for isotropic triaxial loading, 27.9 GPa. At present, we do not have any plausible explanation of this fact.

In Fig. 9(a), it is seen that there are also other extrema of the total energy dictated by symmetry – maxima corresponding to the fcc and sc structures when simulating tensile tests with loading along the [001] and [111] directions, respectively. These extrema are denoted by arrows in Fig. 9(a). Their presence dictates that the corresponding dependence of the energy on elongation must bend, which imposes certain limitations on the maximum stress [22]. In the cases when there is no symmetry-dictated maximum (e.g. in the uniaxial tensile test along the [001] direction of NiAl with the B2 structure in the ground state [24]), the maximum stress is usually higher.

Since the structural energy difference E_{sc}–E_{bcc} is about five times higher than the difference E_{fcc}–E_{bcc} (755 meV/atom compared to 155 meV/atom), the E vs. ε curve for the [111] loading must rise much higher, albeit for larger strains, than that for the [001] loading (see Fig. 9(a)). Consequently, for the tensile test in the [111] direction the inflexion point occurs at a higher strain and for a higher stress than in the test with loading in the [001] direction. Thus, similarly as for W [22], a marked anisotropy of ideal tensile strengths for the [001] and [111] loading directions may be understood in terms of structural energy differences of nearby higher-symmetry structures found at the deformation path.

Relative changes of atomic volume and the dependences of the magnetic moment of FM iron per atom are shown as functions of elongation in Figs. 9(c) and 9(d), respectively. In the neighborhood of the ground state structure the atomic volume increases with increasing elongation but it exhibits a more complex behavior at larger deformations. For isotropic triaxial loading, the magnetic moment shows monotonous increase with increasing volume (in agreement with Herper et al. [95]) while in tensile tests it exhibits local extrema at points corresponding to both higher-symmetry structures (maxima for fcc and simple cubic) as well as at some other points along the paths. Let us note that the increase of the magnetic moment with deformation in the neighbourhood of the bcc ground state in case of uniaxial tensile tests is also connected with increasing volume (cf. Figs. 9(c) and (d)).

5.2. Intermetallic compound Ni_3Al

In contrast to iron, in the case of Ni_3Al we start with the fcc-based $L1_2$ structure and, therefore,

as mentioned in Sec. 2, we renormalize the ratio c/a by ascribing the value of $c/a = 1$ to the $L1_2$ structure. As a result, the c/a for the tetragonal path is by a factor of $\sqrt{2}$ smaller and for the trigonal path by a factor of 4 smaller than in the case of iron.

Using the GGA, the minimum of the total energy is obtained for the ferromagnetic state with the lattice constant equal to 3.561 Å (6.729 au) and magnetic moment of 0.80 μ_B per formula unit. The lattice constant agrees very well with the experimental value [96] of 3.568 Å (6.743 au) whereas the experimental magnetic moment, 0.23 μ_B per formula unit, is much lower. When including the spin-orbital coupling, Xu et al. [97] obtained a value of 0.46 μ_B per formula unit, which is closer to the experimental value. At present, we are verifying this conclusion.

Figure 10 shows the total energy of Ni_3Al as a function of c/a for the trigonal deformation at the experimental lattice volume. This dependence displays a symmetry-dictated minimum at $c/a = 1$ (the ground-state, $L1_2$ structure) and a symmetry-dictated maximum at $c/a = 0.5$ (a sc-based structure exhibiting cubic symmetry). A subsidiary minimum occurs at $c/a \approx 0.27$, which is not dictated by the symmetry. In the structure obtained for $c/a = 0.25$, the atoms are at the bcc-like positions, but the symmetry of this structure remains trigonal.

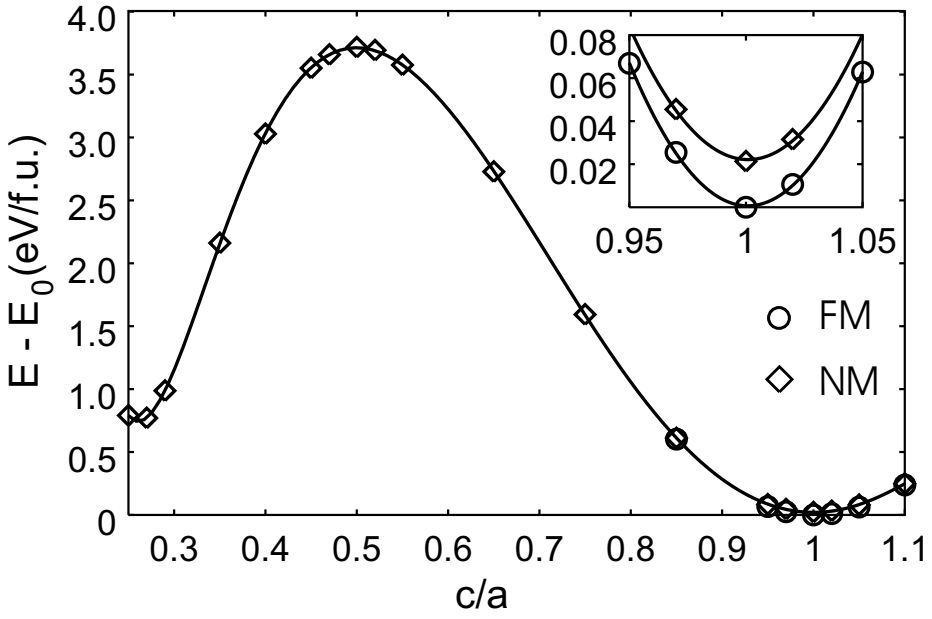

Figure 10: Total energy of Ni_3Al (per formula unit, f.u.) as a function of c/a for the trigonal deformation at the experimental lattice volume. The insert shows the details in the neighborhood of the ground state.

There is a very small energy difference between the FM and NM state of the $L1_2$ structure – only 21.3 meV/formula unit (see the insert in Fig. 10). This is consistent with the results of Xu et al. [97] (0.2-0.5 mRy/f.u.) and Min et al. [98] ($\sim$ 1 mRy/f.u.).

It is seen from Figs. 10 and 11 that the region of existence of FM state is limited. For $c/a \leq 0.75$, the magnetic moment is equal to zero (Fig. 11) and the compound is in a non-spin-polarized state.

Fig. 12 displays the total energy of Ni_3Al as a function of the volume and c/a for the trigonal

deformation. Again, we show only those states the energies of which are the lowest for a given configuration. The total energy profile presented in Fig. 10 is contained in Fig. 12 as a profile for $V/V_{exp} = 1$. A nearly vertical border divides the area of Fig. 12 into FM and NM regions. All energy profiles corresponding to a constant volume exhibit the symmetry-dictated maximum at $c/a = 0.5$. In the contour plot (Fig. 12), there is a saddle point for $c/a = 0.5$ and $V/V_{exp} \sim 1.2$ (outside the area of the figure). The minimum at $c/a \approx 0.27$, $V/V_{exp} \approx 1.01$ is not dictated by symmetry.

Fig. 13 shows the total energy of Ni_3Al as a function of the volume and c/a for the tetragonal deformation. Here NM regions extend to both sides of the FM ground state. However, there are no energy extrema and saddle points in those NM regions. It is interesting that the transition from the FM to NM state during both the trigonal and tetragonal deformation is essentially continuous, without any discontinuities in magnetic moment (see e.g. Fig. 11). Xu et al. [97] have shown that the energy gain in Ni_3Al associated with magnetism is about an order of magnitude smaller than that due to the structural differences. Our calculations show that the NM Ni_3Al in the $L1_2$ structure is stable with respect to tetragonal and trigonal deformations (the shear moduli C' and C_{44} are nearly the same for the NM and FM states). Therefore, magnetism does not appear to play an important role in the control of phase stability. This is in sharp contrast to iron, where the onset of ferromagnetism stabilizes the bcc structure and NM bcc states are not stable with respect to tetragonal deformation [69, 70].

Now, we can also simulate a tensile test in Ni_3Al to get theoretical tensile strengths for uniaxial loading along the [001] and [111] directions. These calculations are presently carried out.

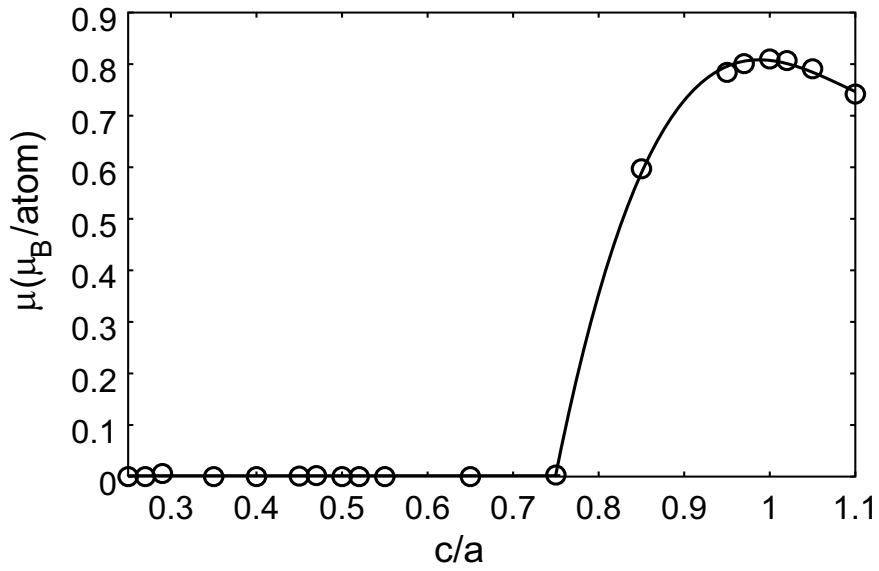

Figure 11: Magnetic moment of Ni_3Al as a function of c/a for the trigonal deformation at the experimental lattice volume.

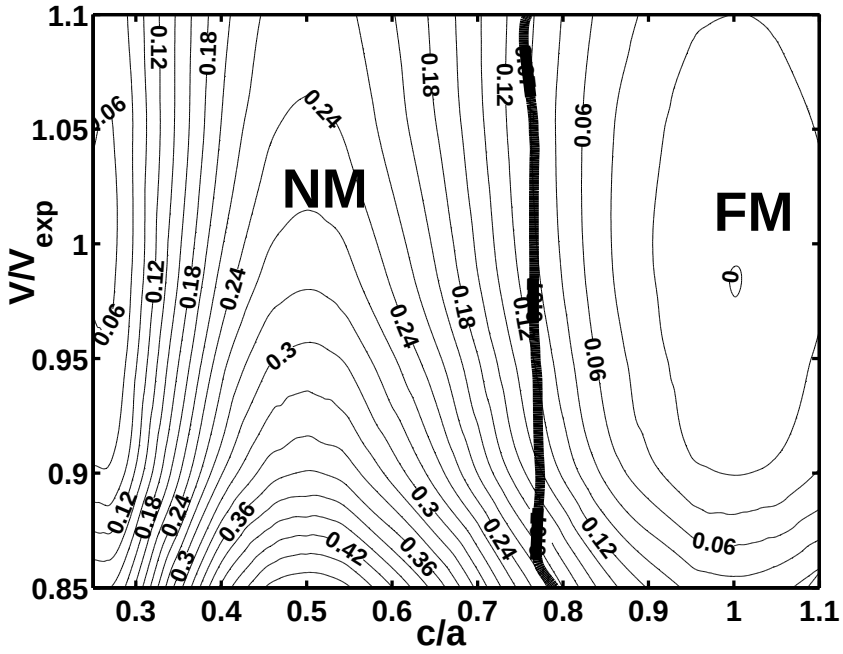

Figure 12: Total energy (per formula unit) of Ni_3Al as a function of volume and c/a ratio, characterizing the trigonal deformation, calculated within the GGA. The energy is measured relative to the energy of the equilibrium FM $L1_2$ state (the minimum at $c/a = 1$). Only states with the minimum energy are shown. The contour interval is 20 mRy. Thick line shows the NM/FM phase boundary. The ground-state minimum at $c/a = 1$ and the saddle point at $c/a = 0.5$ and $V/V_{exp} \sim 1.2$ (outside the figure area) are dictated by symmetry.

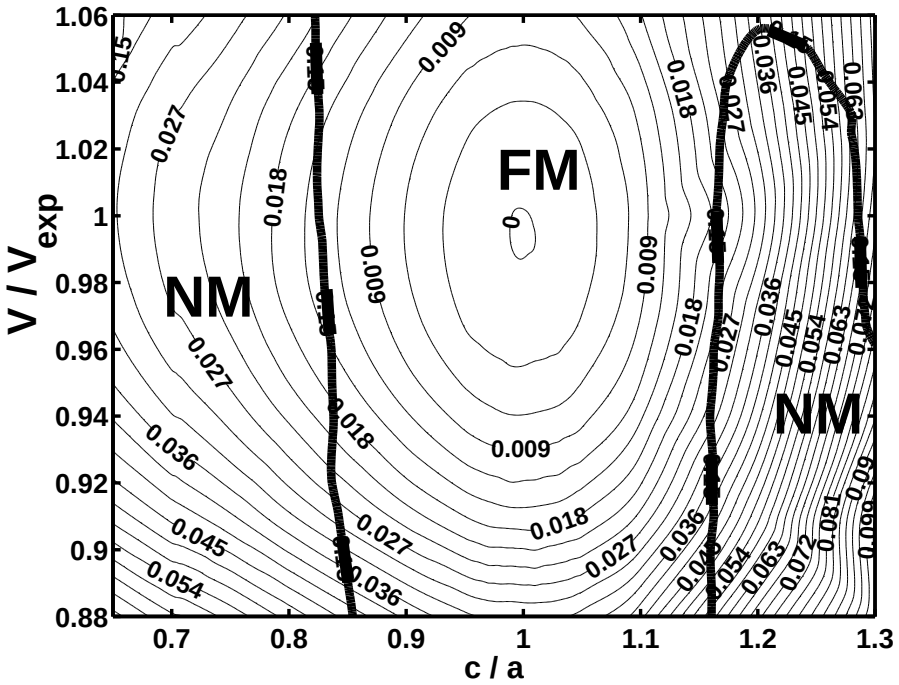

Figure 13: Total energy (per formula unit) of Ni_3Al as a function of volume and c/a ratio, characterizing the tetragonal deformation, calculated within the GGA. The energy is measured relative to the energy of the equilibrium FM $L1_2$ state (the minimum at $c/a = 1$). Only states with the minimum energy are shown. The contour interval is 3 mRy. Thick lines show the NM/FM phase boundaries. The only symmetry-dictated extremum is at $c/a = 1$.

6. Ab initio calculated values of theoretical tensile strength

For the sake of completeness, we summarize in the Table 1 all ab initio calculated values of the theoretical tensile strength (including relaxation in directions perpendicular to the loading axis and, if applicable, of internal structure parameters) that have been calculated until now. Most of them correspond to the inflexion point on the strain dependence of the total energy. Non-relaxed calculations are also included; th ecorresponding values are denoted by a dagger (†). As for the strength of W for [110] loading, the material probably breaks down due to some other instability before reaching the inflexion point and, therefore, the true theoretical tensile strength will be lower than that given in the Table. The situation is most likely the same in the case of Cu where the experimental ideal strengths are about an order of magnitude lower than the calculated ones [25, 99]. Semiempirical calculations [87] indeed suggest that, for the [001] direction, the tetragonal shear modulus becomes zero well before reaching the inflexion point. It may be expected that similar instabilities will occur for the [110] and [111] orientations. This will be the subject of further investigations.

7. Conclusions

We analyzed the energetics of iron and the intermetallic compound Ni_3Al subjected to tetragonal and trigonal deformation by means of full-potential ab initio electronic structure calculations and found borders between various phases with different spin polarizations. Whereas in iron the magnetic effects are vital for understanding the deformation behaviour and a variety of magnetic orderings occurs, it transpires that in Ni_3Al magnetism is not very important in phase stability considerations. The $L1_2$ ground state is ferromagnetic, but the energy difference between the FM and NM state is quite small, about 21 meV/formula unit. It is interesting that during tetragonal deformation, iron transforms to AFMD and AFM1 states (Fig. 5), whereas during trigonal deformation, it is mostly ferromagnetic (Fig. 6).

For iron, we analyzed uniaxial tensile tests and discussed the anisotropy of the theoretical tensile strength, namely 12.7 GPa for [001] and 27.3 GPa for the [111] direction of loading. This marked anisotropy may be understood in terms of the symmetry-dictated extrema that are present along the deformation paths. Also the isotropic triaxial (hydrostatic) tension was analyzed and theoretical tensile strength of iron for this mode of loading was found to be 27.9 GPa, very close to the value for uniaxial [111] loading.

It should be noted that the calculated dependence of the total energy on parameters of the transformation paths provides useful information when constructing semi-empirical interatomic potentials that may be used for computer simulation of atomic configurations of various extended defects for which the first-principles calculations are intractable. An example is bond-order potentials (BOPs) [100] for which we have shown recently how such first-principles results may be employed in their construction and testing [92, 101].

Stability of higher-energy structures is also an important issue in the theoretical basis of the CALPHAD (CALculation of PHAse Diagrams) method [102]. Grimvall [103, 104] concludes that when either the bcc or fcc structure of a metal is dynamically unstable, i.e. unstable, for example,

material	structure	direction	σ_{th} (GPa)	reference
Fe	A2	[001]	12.7	[57, 59]
		[001]	14.2	[58]
		[111]	27.3	[59]
W	A2	[001]	28.9	[22]
		[001]	29.5	[32]
		[111]	40.1	[22]
		[110]	54.3	[22]
Al	A1	[001]	12.1	[26]
		[111]	11.05	[26]
		[111]	11†	[27, 28]
Cu	A1	[001]	55†,32†	[13]
		[001]	33	[25]
		[110]	31	[25]
		[111]	29	[25]
diamond	A4	[111]	90	[35]
		[111]	95	[36]
		[001]	225	[35]
		[110]	130	[35]
Si	A4	[111]	22	[36]
Ge	A4	[111]	14	[36]
Nb	A2	[001]	13.1	[37]
Mo	A2	[001]	28.8	[37]
TiC	B1	[001]	44	[21]
NiAl	B2	[001]	46	[24, 25]
		[111]	25	[24, 25]
β-SiC	B3 (3C)	[001]	101	[34]
		[111]	50.8	[34]
AlN	B4	[0001]	50†	[27, 28]
$MoSi_2$	$C11_b$	[001]	37	[55, 56]
WSi_2	$C11_b$	[001]	38	[55, 56]
β-Si_3N_4	$P6_3/m$	[100]	72.2†	[38]
		[100]	57	[40]
		[001]	75.0†	[38]
		[001]	55	[40]
c-Si_3N_4	$Fd\bar{3}m$	[001]	45	[39]

Table 1: Theoretical tensile strengths σ_{th} calculated ab initio. The dagger means that the perpendicular dimensions of the sample were not relaxed during the calculations (no Poisson contraction allowed).

with respect to the tetragonal or trigonal deformation, then there are large discrepancies between the semiempirical enthalpy differences H_{bcc}-H_{fcc} obtained from the CALPHAD method and ab initio results. However, as we can see from Refs. [16, 18, 81], this is the case in most transition metals. In ab initio calculations, the dynamical instability is suppressed since we impose a rigid lattice (in reality, this might be stabilized by some external constraints), and the energy and enthalpy of such structure have well defined physical meaning. However, it appears that it is not certain how such values may be compared with those obtained from semiempirical CALPHAD method.

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