Ψ_k Newsletter

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

Number 64   August 2004

Contents

1 Editorial

The summer season is reflected in this newsletter through a reduced number of contributions. However, we encourage our readers to respond to the call for suggestions on symposia and speakers for our 3rd Psi-k Conference, i. e., Psi-k2005 which will be held on 17-21 September, 2005 in Schwäbisch Gmünd, Germany, the usual place of the Psi-k conferences.

The announcement of the mid-term review meeting and workshop to be held in Paris on 8-10 December, 2004 can be found in the RTN2 "f-Electron Materials" section. In the ESF Programme section the chairman, Prof. dr Peter Dederichs, writes about the joint EC-NSF activity and repeats the call for workshop proposals for 2005. In this section there is also a detailed report on the recent ABINIT workshop. Another workshop report can be found in the section of the UK CCP9 Programme. Job and general conference announcements, as well as abstracts of newly submitted papers are placed in their usual sections. This issue's scientific highlight is by J. Kioseoglou, G.P. Dimitrakopulos, Ph. Komninou, H.M. Polatoglou and Th. Karakostas (*Thessaloniki*) on **"Partial dislocations in wurtzite GaN"**. 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 2004 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@dl.ac.uk	**messages to the coordinators, editor & newsletter**
psik-network@dl.ac.uk	**messages to the whole Ψ_k community**

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

2 General News

2.1 Psi-k2005 Conference

Towards Atomistic Materials Design
Schwäbisch Gmünd

17-21 September, 2005

Call for Suggestions

This is to encourage you all to submit your suggestions for topical symposia as well as plenary and symposia speakers for the Psi-k 20005 Conference. The suggestion form will be available on the conference web page

http://www.fyslab.hut.fi/psik2005

at the end of August. In the meantime the suggestions may be sent by e-mail to Marko Rusanen (mtr@fyslab.hut.fi).

Please spare some time and fill in the suggestion form for the symposia and speakers or send them to Marko by e-mail. We would appreciate very much if you could do this as soon as possible. We would like to take into account everybody's input while formulating a preliminary programme of the Conference for discussions with the Programme Committee and the International Advisory Committee.

If you encounter any problems with accessing the above web page or have any questions regarding suggestions, please contact Marko Rusanen (mtr@fyslab.hut.fi) by e-mail.

Thank you,

Z. (Dzidka) Szotek   Risto Nieminen (Conference Chairman)
psik-coord@dl.ac.uk   rni@fyslab.hut.fi

3 News from the RTN2 Network

”f-Electrons Materials”

3.1 RTN2 Workshop Announcements

3.1.1 Workshop and Mid-term Review of the RTN ”f-Electron Materials”

”Electronic Structure of Correlated Materials”

Institut Henri Poincaré, Paris, France

8-10 December, 2004

Organizing Committee:

Silke Biermann
Antoine Georges
Erich Wimmer

The web page of the above meeting is

http://www.cpht.polytechnique.fr/ihp2004.html.

Please check the above for details.

The deadline for registration is 1 November, 2004.

4   News from the ESF Programme

"Towards Atomistic Materials Design"

4.1   Information on a Joint EC-NSF Activity in Computational Materials Research

We would like to point your attention to a new EC-NSF coordinated call for collaborative projects between EU and US scientists in Computational Materials Research. The objective addresses "properties and phenomena that span multiple time and length scales" and covers a broad range of areas in computational materials science such as crystal growth, ..., grain boundaries, spintronics and molecular electronics, etc.

Information on the call can be obtained from the cordis web site:

`http://fp6.cordis.lu/nmp/call$\_$details.cfm?CALL$\_$ID=135`

Identifier: [FP6-2004-NMP-NSF-1]

Closing date for applications is 14 October 2004.

Each proposal should include, on both sides of the atlantic, at least 3 teams. The joint proposal will be independently reviewed by the NSF and the EU. This call should be of strong interest for a large number of groups. However only about five proposals will be funded.

There was an introductory NSF/EC workshop on "Methods in Computational Materials Science" at the MRS Spring Meeting 2004 in San Francisco, where interesting scientific topics have been identified. The report is available on the web (www.itamit.dtc.umn.edu/nsfreport.php). However in the end, the text of the above call is decisive.

Peter H. Dederichs
(Chairman, Psi-k Programme)

4.2 Call for Workshop Proposals for 2005

There will be no support for workshops in 2005 because of our own Psi-k2005 Conference on 17-21 September 2005, but instead people are encouraged to submit ideas for invited speakers grouped into a symposium at the conference: see call for suggestions in August or October Newsletter.

However support for hands-on tutorials and perhaps one or two other activities not conflicting with the conference may be considered.

A proposal should be submitted by email (in the form of a single simple email letter WITHOUT ATTACHMENTS OR LATEX, just plain ASCII) to the Psi-k Programme secretary, Walter Temmerman, at

<div align="center">psik-coord@dl.ac.uk</div>

by 15 September 2004 as absolutely final deadline.

The proposal should include the following points (preferably numbered in this order).

1. Title and purpose of the event, with names and addresses (including email) of the organisers.

2. The scientific content and why this event would be useful at this time.

3. A tentative list of speakers whom it is hoped to have.

4. The number of participants it is planned to invite or attract, and their scientific involvement, e.g. as simulators, related experimentalists, code developers, etc., and young scientists in the subject.

5. Plans for a tutorial element and for attracting new researchers into the subject of the workshop. (If this is thought inappropriate for this workshop, please explain why.) The purpose of the ESF Psi-k Programme is to help everyone in our community to do good quality research, and in our expanding field this implies some outreach and tutorial activity.

6. Budget, expressed in Euro, and how much is being applied for from the ESF Psi-k Programme. In the past, this has been limited to about 9k Euro.

7. A statement about other organisations which will be applied to for co-sponsorship and additional funding, e.g. any EU RTN Network, CECAM, CCP9 in the UK, etc..

8. Where it is hoped the event would be held.

9. Plans about inviting and financing any participants from countries outside Europe including America and Japan.

Peter Dederichs
Chairman of ESF Psi-k Programme

Workshop ABINIT 2004
Paris, May 10-12, 2004

Summary

The abinit workshop took place on the 10-13 may 2004, at the Carr de sciences in Paris. The main theme of the workshop was to review progresses made during the last 18 months, in particular the new computational capabilities offered in the field of electronic structure by the Abinit code. Two additional days were devoted to a "coding party", that is, developping small pieces of software or discussing future directions.

The workshop was attended by 46 people, all invited, from many european coutries (but principally France and Belgium) and also from the U.S., Canada and Japan. The coding party was smaller in size, with about 10 people attending.

In the realm of methodology, work on the PAW (projected augmented wave) method, the calculation of elasticity coefficients by linear response, the determination of electron phonon coupling coefficients, and non-linear electric and optical properties were most prominent ones.

Tha PAW method is now completely implemented as for total energy calculation, using either Vanderbilt's ultra soft pseudopotential generator, or the generator of N. Holzwarth.

The calculation of elasticity coefficients by linear response was a tour de force by Don Hamman (its inclusion created a discontinuity in the code's length statistics). This calculation made a heavy use of the tensorial structure of Abinit (based on Legendre polynomials) for the calculation of non local operator (which is present in parallel with the more traditional spherical harmonics expansion, necessary for PAW). and a technical discussion took place on the convention used for the elasticity coefficients at finite pressure. A note about this has been written directly in the Infos files.

The calculation of non-linear propertie necessitate the third-order energy derivatives with respect to three electric fields and two electric fields and one atomic displacement by making use of the 2n+1 theorem in the line of Nunes and Gonze. One can in this way compute the Raman susceptibilies of transverse and longitudinal optical phonons and the electrooptic coefficients. In the same vein, two methods for the first-principles calculation of insulators in a finite electric field and their implementation in the ABINIT code were presented.

The first method allows to compute the structural response of a periodic insulating solid to a homogeneous static electric field within density functional perturbation theory (DFPT). The second technique consists in iteratively minimizing an electric field dependent energy functional

On the software engineering side, the use of XML markup langage for structuring I/O (in agreement with the CML (Chemical Markup Langage) one of the de facto norm), the content and aspect of the WEB site and the use of NetCDF for very large arrays were presented.

An analysis of the statistics of the code revealed also that the numbers of lines as well as the number of test cases is roughly linearly increasing since 4 years, as well as that most european registrered in the user's list come from Germany while most developper's come from Belgium and France (the CEA in particular).

Finally, some users were invited specifically because their applications were demanding new directions (electronic excitations, conjugate polymers, growth mechanisms or surface and molecular crystals)

Two open discussions took place:

1) Research contracts

The objective was mainly to connect software developpements projects (like Abinit) and European research grants in order to enhance each other.

2) Debriefing and future plans

We decided to propose a user's tutorial alongside the March meeting to be held in San Francisco next year, and the next developper's workshop within two years.

Finally, during the two final days, we discussed NetCDF (for wave function files), enhancement of documentation and restart files (that is a density file every N steps). This last item was partially implemented.

In conclusion, the progress made in the Abinit software were sustained during the last 18 months, and its scope of applications, which encompass ground state properties (with optimisation of structure and molecular dynamics) linear response with much work on second order linear response, and optical properties are still going to be extended in the direction of using softer pseudo potentials, new algorithmes in general, massive parallelisation and more elaborate treatment of I/O for analysis.

A complete set of presentation slides can be found on the workshop's web site at:

http://www.abinit.org/workshop/present.html

Program

MONDAY (May 10)

SESSION I : INTRODUCTIVE SESSION (Chair : D.C. Allan)

10:30: Welcome Gilles ZERAH

10:40 (15'+5') **ABINIT : 3.5 years of GNU GPL Licence** Xavier GONZE

11:00 (25'+10') **Electronic Excitations of Cu2O within GW Approximation** Fabien BRUNEVAL

11:35 (30'+10') **Organization of software for the computational design of new materials** Nicola SPALDIN

12:15 Lunch

SESSION II : NEW FEATURES: GROUND STATE (Chair D.R. Hamann)

14:00 (30'+10') **PAW Atomic Data Generation for ABINIT** Marc TORRENT

14:40 (30'+10') **Implementation of the PAW formalism in ABINIT : present features and perspectives** Franois JOLLET

15:20 Coffee Break

15:50 (15'+5') **DOS and partial DOS in ABINIT: angular momentum projection and the tetrahedron method** Matthieu VERSTRAETE

16:10 (30'+10') **Experimentation with parareal molecular dynamics and Thomas-Fermi as a predictor** Gilles ZERAH

16:50 (20+10') **Parallel research of numerous eigenvalues in ABINIT** Christophe AUDOUZE

TUESDAY (May 11)

SESSION III : SOFTWARE ENGINEERING (Chair F. Jollet)

9:00 (40'+10') **XML in ABINIT** Xavier GONZE

9:50 (30'+10') **CMLComp : an XML.CML infrastructure for computational chemistry** Peter MURRAY-RUST

10:30 Coffee Break

11:00 (15'+5') **Debian and RPM packages for ABINIT** Yann POUILLON

11:20 (10'+20') **The ABINIT Web SITE and MAILING LISTS** Jean-Michel BEUKEN

11:50 Lunch

SESSION IV : NEW FEATURES: LINEAR AND NON-LINEAR RESPONSE (Chair G.-M. Rignanese)

14:00 (30'+10') **First-principles study of periodic solids in a finite electric field** Marek VEITHEN

14:40 (40'+10') **Implementation of the Strain Perturbation in ABINIT** D.R. HAMANN

15:30 Coffee Break

16:00 (25'+10') **The electron-phonon interaction in ABINIT** Matthieu VERSTRAETE

16:35 (30'+10') **Computation of non-linear optical properties from density functional perturbation theory** Marek VEITHEN

17:15 Discussions on: "Research contracts and possible financements" (Chair : D.C. Allan)
With Thierry Deutsch (BIGDFT project), Philippe Ghosez (FAME project), Yann Pouillon and Florent Tournus (EXCITING network), Lucia Reining (NANOQUANTA project)

WEDNESDAY (May 12)

SESSION V : APPLICATIONS (Chair N. Spaldin)

9:00 (25'+10' **ABINIT applications / Rare-earth Sesquioxides/oxysulfides and a photochromic Molecular Crystal** Masayoshi MIKAMI

9:35 (25'+10') **Elementary growth mechanisms in magnesium oxide (001) HOMOEPI-TAXY : from the isolated adssorbates to the complete monolayer** Grgory GENESTE

10:10 Coffee Break

10:40 (25'+10') **Design of novel conjugated polymers based on fluorene, carbazole and borafluorene** Michel COTE

11:15 (25'+10') **Ab initio phase diagrams of minerals** Artem R. OGANOV

11:50 Lunch

SESSION VI : SOFTWARE ENGENEERING AN CONCLUDING SESSION (Chair : G. Zerah)

14:00 (30'+10') **NetCDF, one answer to data portability nightmare** Jean-Paul MINET

14:40 (30'+10') **NetCDF implementation in molecular dynamic** Muriel DELAVEAU

15:20 **Strategic discussions and Debriefing of the workshop Planning of the next workshop**

16:00 Departure Coffee break

Abstracts

Parallel research of numerous eigenvalues in ABINIT

Francois Alouges and Christophe Audouze

Laboratoire de Mathématique, UMR CNRS 8628, Université Paris-Sud, Bâtiment 425,
F-91405 Orsay Cedex

In ABINIT, the research of N orthonormal wave functions for the Kohn-Sham model is associated with an algorithm which owes a $O(N^3)$ complexity. We propose a new parallel algorithm, based on a spectral partitionning of an energy band which is to be determined. We calculate independently clusters of eigenvalues with local orthogonalizations. We give a partitionning criterium of the energy band adapted to the kind of eigenvalue algorithm used. In collaboration with the CEA, this method should lead to an algorithm of complexity $O(N^2)$ in the ABINIT project.

The ABINIT Web Site and Mailing Lists

Jean-Michel Beuken

Unité de Physico-Chimie et de Physique des Matériaux,
Université Catholique de Louvain,
1 Place Croix du Sud, B-1348 Louvain-la-Neuve, Belgium

Electronic Excitations of Cu_2O within GW Approximation

Fabien Bruneval, Nathalie Vast, Lucia Reining, and Valerio Olevano

Laboratoire des Solides Irradis - CEA/CNRS/Ecole Polytechnique - 91128 Palaiseau

Cuprous oxide has been extensively studied during the last decades, mainly because of its exciton series in the optical range. Cu_2O is a good starting point to address the fundamental issue of transition metal oxides. Indeed, this material has a cubic structure, a closed d shell, and is non-magnetic. The topic of transition metal oxides is now very important: it is known that density functional theory fails to predict a gap in various insulating oxides like CoO, CuO, Ti_2O_3.

We performed DFT and GW calculations using ABINIT package. We carefully studied the role of semicore states ($3s^2 3p^6$). Though deep in energy, these states have a large overlap with valence bands. Their influence is slight on the Kohn-Sham band structure. However, we state that the semicore states have to be included in the GW calculation to get meaningful results.

Even a GW calculation including semicore states largely underestimates the quasiparticle gap. Further approximations are used to conduct a "standard" GW calculation, as in ABINIT code: the use of a plasmon pole model, a first order perturbation scheme, etc.

We extensively discuss many of them and conclude that they are reliable. Then the failure of GW may lie in the neglect of vertex functions.

Design of novel conjugated polymers based on fluorene, carbazole and borafluorene

Michel Côté and Jean-Franois Brière

Département de physique, Université de Montréal et Regroupement québécois sur les matériaux de pointe (RQMP)

In this presentation, I will show the results of our investigation of conjugated polymers using ABINIT, an application in the design of novel materials. The discovery, in the early 1990's, of the blue electroluminescence of poly-(para-phenylene)(PPP) stimulated the interest given to conjugated polymers for materials employed in electronic devices. In addition to their use in light emitting diodes and possibly in lasers, some derivatives of PPP with smaller energy gaps seemed like they might be good candidates for technological innovations such as organic photovoltaic devices used to convert solar energy and all organic transistors. Theoretical studies of the single stranded polymers based on fluorene, carbazole and borafluorene indicate that they exhibit many common features, such as their wave functions, even if the presence of nitrogen or boron atom modifies some properties, like the minimum energy gap which is considerably smaller for poly(2,7-borafluorene). In order to further decrease the energy gaps, it is interesting to consider the ladder-type polymers based on the molecules mentioned. The planarity of these polymers favors the alignment of some critical π-orbital that should results in smaller energy gaps.

NetCDF implementation in molecular dynamic of ABINIT: An example of interfacing netCDF data with the interacting plotting program xmgrace

Muriel Delaveau, Jean Clerouin, Bernard Magne, and Gilles Zerah

CEA/DPTA/SPMC, Ile de France, 91680 Bruyères-le-Chatel

The implementation of netCDF in the aim of storing molecular dynamics data in a portable way is presented. An example of interfacing netCDF data with the interacting ploting program xmgrace is given. The interface has been writtent in Python, using K. Hinsen's ScientificPython package.

Elementary growth mechanisms in magnesium oxide (001) homoepitaxy : from the isolated adsorbates to the complete monolayer

Gregory Geneste[1], Joseph Morillo[2], Fabio Finocchi[3], Marc Hayoun[4]

[1] *Universit de Lige, Institut de Physique, Alle du 6 Aout 17, B-4000 Sart Tilman, Belgium*

[2] *Centre d'Elaboration de Matriaux et d'Etudes Structurales, CNRS UPR 8011, 29 rue Jeanne Marvig, BP 4347, 31055 Toulouse Cedex 04, France*

[3] *Groupe de Physique des Solides, CNRS UMR 7588, Campus de Boucicaut, 140 rue de Lourmel, 75015 Paris, France*

[4] *Laboratoire des Solides Irradis, CEA/DSM/DRECAM, CNRS UMR 7642, Ecole Polytechnique, 91128 Palaiseau Cedex, France*

Metal oxides are used in a wide range of applications, as epitaxially grown thin films, as substrates, or both of them. Beyond its fundamental interest, the understanding of the basic growth mechanisms is therefore important for a better control of the growth process itself. We focus on MgO(001) growth, mainly studied by means of DFT simulations (within the ABINIT code), performing an overall study of the elementary processes, considering the Mg and O atoms, and the O_2 molecules as the deposited species, as it occurs in molecular beam epitaxy or sputtering.

We show that on the surface, Mg and O behave differently, the local electronic and atomic structures playing a crucial role in determining the energy landscape seen by the diffusing species : whereas on the flat surface only Mg can diffuse easily, the situation is reversed along the $\langle 001 \rangle$ step. The peculiar natures of the substrate-adsorbate chemical bonds are responsible for these differences.

Sticking together, adsorbed Mg and O atoms eventually form magnesium oxide : the study of the various redox reactions between the ad-species reveals that the actual surface stoichiometry results from a subtle interplay between their reactivity and diffusing behaviour. The Mg + O → MgO surface reaction must proceed, for example, with a strong local rearrangement. We show that this reaction occurs without any extra barrier than that for Mg diffusion. We also study the molecules and clusters, products of this redox process, and show that nucleation centers appear at very small sizes. The way they enlarge by adsorbing diffusing species is investigated, up to the complete monolayer. We show for instance that cluster edges and steps attract Mg adatoms, and explain why $\langle 110 \rangle$ edges are unstable, reflecting the existence of a destabilizing macroscopic electric dipole.

Finally, we outline a possible scenario for large-scale homo-epitaxy with particular emphasis on the perspectives of linking our atomic-scale calculations to the macroscopic models that are

commonly used to describe crystal growth. In particular, we show that those models must be generalised to account for the larger complexity of the chemistry and electrostatics at oxide surfaces, compared to elementary metals.

XML in ABINIT

X. Gonze

Unité de Physico-Chimie et de Physique des Matériaux,
Université Catholique de Louvain,
1 Place Croix du Sud, B-1348 Louvain-la-Neuve, Belgium

In the first part of the talk, an introduction to the basic concepts of XML (the eXtensible Markup Language) will be given.

Then, the present use of XML in ABINIT will be briefly described : I/Os using CML, a "flavor" of XML ; the inclusion of the XMLF90 library, from A. Garcia.

The future of XML in ABINIT will then be discussed.

ABINIT : 3.5 years of GNU GPL licence

X. Gonze

Unité de Physico-Chimie et de Physique des Matériaux,
Université Catholique de Louvain,
1 Place Croix du Sud, B-1348 Louvain-la-Neuve, Belgium

In this brief talk, a summary of the evolution of the ABINIT project in the recent years will be presented.

Implementation of the Strain Perturbation in ABINIT

D. R. Hamann[1,2,3], Xifan Wu[1], David Vanderbilt[1], Karin Rabe[1]

[1] *Department of Physics and Astronomy, Rutgers University, Piscataway, NJ, USA*

[2] *Bell Laboratories, Lucent Technologies, Murray Hill, NJ, USA*

[3] *Mat-Sim Research LLC, Murray Hill, NJ, USA*

The strain perturbation has been incorporated into the response function (RF) capabilities of ABINIT, allowing the direct calculation of the elastic, piezoelectric, and internal strain tensors. Following a brief review of density functional perturbation theory, we will show how the pervasive internal use of reduced coordinates in ABINIT permits strain to be systematically treated like any other perturbation. The extensive changes to the RF code (29 new and 24 modified routines) will be outlined and classified within a schematic summary of the code structure. For the benefit of future developers, we will describe the process of this development effort in some detail, and the considerations motivating certain choices made along the way. The RF strain results represent rigid-ion quantities. We have added functionality to anaddb to post-process these results together with existing interatomic force constants and Born effective charges to yield the physical relaxed-ion quantities. The use of all these capabilities will be illustrated. We will conclude with an assessment of future developments, including anticipated benefits and pitfalls

Implementation of the PAW formalism in ABINIT: present features and perspectives

F. Jollet, M. Torrent, F. Bottin, and G. Zerah

Commissariat à l'Energie Atomique, Centre d'Etudes de Bruyères-le-Chatel, BP 12, F-91680 Bruyères-le-Chatel

In this presentation, we shall review all the new features added since the first ABINIT workshop. We shall especially focus on the following points:

- What has been added or modified for PAW implementation?

- How does a PAW calculation work?

- What about accuracy and efficiency?

- Physical examples

ABINIT applications : Rare-earth Sesquioxides/Oxysulfides and a photochromic Molecular Crystal

Masayoshi Mikami and Shinichiro Nakamura

Mitsubishi Chemical Group Science and Technology Research Center, Inc., 1000, Kamoshida-cho, Aoba-ku, Yokohama 227-8502, Japan

Several ABINIT calculations have been performed as useful benchmarks to probe the feasiblity and limit of the code.

The first example is a calculation of rare-earth sesquioxides R_2O_3 and oxysulfides R_2O_2S (R=La, Ce, and Pr, Space Group 164). By adopting rare-earth pseudopotentials with their 4f-states as

core electrons, equilibrium atomic geometries, band structures, bulk moduli, Raman/IR vibration modes and dielectric properties are successfully evaluated within the local density approximation of density functional theory. The comparison with experimental data appears so good that the rare-earth pseudopotentials may be applied to other rare-earth insulators, although electronic excitations cannot be discusseed.

The second example is a calculation of salicylideneaniline molecular crystals, in which tautomerization reactions involving intermolecular hydrogen bonds take place under photoirradiation. Evaluated dielectric permittivity tensors of the molecular crystals indicates that the photo-driven tautomerization reaction induce sufficient change of the refractive indices advantageous to various applications such as photochromic memory or switch [1].

Possible functions in future ABINIT will be suggested on the basis of the present benchmarks.

[1] M.Mikami and S.Nakamura, Phys.Rev.B69, 134205 (2004).

NetCDF, one answer to data portability nightmare

Jean-Paul Minet

Institut de calcul intensif et de stockage de masse, Univeristé Catholique de Louvain, Belgium

The netCDF libraries define a machine-independent format for representing scientific data. Together, the interface, libraries, and format support the creation, access, and sharing of scientific data.

By nature, NetCDF data is:

- Self-Describing: a netCDF file includes information on the data it contains.

- Architecture-independent: a netCDF file is represented in a form that can be accessed by computers with different ways of storing integers, characters, and floating-point numbers.

- Direct-access: a small subset of a large dataset may be accessed efficiently, without first reading through all the preceding data.

Throughout this talk, we will be looking at the problems involved in portability of binary data, presenting netCDF concepts and detailing a couple of often used netCDF functions.

CMLComp: an XML.CML infrastructure for computatational Chemistry

Peter Murray-Rust

University of Cambridge

CML is now the de facto approach for representing chemistry in XML. Recently we have developed CMLComp to support a wide range of computational chemistry tasks and concepts. An important principle is that all concepts must be easily and robutly implementable at low cost. We have therefore developed an infrastructure which allows machine generation of much of the code. This has been recently presented to the UK and other eScience communities and a distribution made available [1]. All material is Open source and intended for wide redistribution.

An important central philosophy is to develop components for computational chemistry. This has several benefits:

- quality is increased

- semantics of operations are clearer

- data types can be shared by the community

- modular designs can be created where components from different suppliers (e.g. different codes) can be linked

- high-throughput computing can be managed robotically.

- workflows for the GRID can be packaged and distributed

We have demonstrated proof-of-concept by running and analysing 750000 semi-empirical computational chemistry jobs (ground state optimisation of small covalent molecules in gas phase). Results are in XML/CMLComp and are stored in an XML database. This is searchable by ID, exact chemical species and calculated properties. The results can be fed into more expensive methods if required.

A central approach is that each computational code can be customised to fit this model. Code authors need to:

- identify the input concepts in their code (data, control, methods, parameterisation, etc.)

- identify the output concepts (properties, job information, etc.)

- map them onto dictionaries for CMLComp concepts. Where these do not exist create their own dictionary. We expect to see code-specific dictionaries for all major packages with linkage to commonly agreed terms.

- either create XML/CML readers for the input concepts

- or create XSLT stylesheets to create native program input

- either create XML/CML writers for the output concepts

- or use a parser to transform native program output into XML/CMLComp

Ideally code authors would:

- create an XML dictionary of terms used in the program.

- create input methods for the program

- add XMLwriters to the code

We have libraries for XML input and output for common languages. Java is best developed, then C++ and Python (wortk required). Fortran is at proof-of concept.

For closed codes the last two operations and managed by "wrapping" the code as above but it is less satisfactory.

The ABINIT workshop gives an excellent opportunity to make a start on communal dictionaries and to XMLise some or all of the code.

[1] http://wwmm.ch.cam.ac.uk/moin/CmlAtNesc (includes a 80 Mbyte distribution)

Ab initio phase diagrams of minerals

Artem R. Oganov[1], Shigeaki Ono[2], G. David Price[3], Michael J. Gillan[3]

[1] *Lab. of Crystallography, Dept. of Materials, ETH Zurich, Zurich 8092, Switzerland. E-mail: a.oganov@mat.ethz.ch.*

[2] *Institute for Frontier Research on Earth Evolution, Japan Marine Science & Technology Center, 2-15 Natsushima-cho, Yokosuka-shi, Kanagawa 237-0061, Japan.*

[3] *University College London, Gower St., London WC1E 6BT, U.K.*

The last decade has seen a dramatic increase in the capability of ab initio simulations and their applicability to geologically relevant problems. One of the most pieces of information that is difficult to obtain experimentally at high pressure is the phase diagram: phase diagrams of Earth-forming systems determine the structure and dynamics of our planet, as well as chemical processes within it. Density-functional perturbation theory provide the most straightforward route to calculating free energies of solid phases and constructing phase diagrams.

Theoretically calculated phase diagrams of MgO and SiO_2, along with results on the possible decomposition of $MgSiO_3$ perovskite into $MgO + SiO_2$ in the lower mantle and post-perovskite phases of $MgSiO_3$, will be presented. Our results resolve some of the long-standing controversies in deep mantle mineralogy, such as stability of $MgSiO_3$ perovskite and phase relations in SiO_2 at megabar pressures. Comparison with the latest experiments is very favourable.

Debian and RPM packages for ABINIT?

Y. Pouillon and X. Gonze

Unité de Physico-Chimie et de Physique des Matériaux,
Université Catholique de Louvain,
1 Place Croix du Sud, B-1348 Louvain-la-Neuve, Belgium

As ABINIT is growing both in popularity and in size, it could take a lot of benefit from following more standard package maintenance and distribution guidelines. They could not only ease the tasks of the developers and maintainers but also provide the end-users with a more friendly and well-established way to obtain executables optimized for their needs, as well as more easily installable.

Since ABINIT is a free software project, the first natural step is to add support for the GNU Autotools (mainly Autoconf, Automake, and Libtool) which enable the automatic production of Makefiles after an comprehensive detection of the relevant platform parameters. This had been tentatively developed for the 3.x versions and we have restarted from scratch on top of the 4.3.3 version.

Once there is a reliable support for the GNU Autotools it would be straightforward to build Debian and RPM packages.

However these enhancements raise a certain number of issues.

First of all the GNU Autotools strongly recommend to respect the GNU Coding Style — what ABINIT does not at this point — announcing that this policy will be reinforced in their next versions. Conformance to these rules requires changes in the directory tree structure.

Furthermore most of these rules become mandatory for Debian and RPM packages, in addition to even stronger requirements.

Along with the binary packages one will have to provide the end-user with selected data too, since ABINIT needs at least pseudopotentials for "ordinary" operations. This means auxilliary packages, file location policies, and strict naming conventions.

The evolution of ABINIT towards the distribution of prepackaged binary versions implies philo-sophical as well as practical and technical questions which have to be extensively discussed among the community of ABINIT users and developers.

That is why we propose a smooth-transition strategy until all these developments come to sufficient maturity.

Organization of software for the computational design of new materials

Nicola Spaldin

Materials Department, University of California, Santa Barbara, CA 93106-5050, USA

This talk describes the somewhat disorganized state of computer software in a typical University research program (my own) to advocate for more coordination between the various large code development groups. Our research studies the fundamental physics of a range of novel materials including multiferroics (which are simultaneously ferromagnetic, ferroelectric and ferroelastic),

magnetic semiconductors and materials for molecular spintronics. The questions we investigate are varied and require a range of tools, and we are currently using the following software packages:

- ABINIT, for its linear response capability

- SIESTA, since the local orbital basis set allows us to study large systems

- an in-house ultra-soft pseudopotential code which we have modified to include self-interaction corrections to the exchange-correlation functional

- the Stuttgart-LMTO package, for its visualization tools, and

- VASP, for its speed and LDA+U capabilities.

We outline some of the factors, both technical and historical, that have led to this untidy diversification and suggest some ideas for future improvement. Finally we describe one application, the investigation of grain boundaries in cobalt-doped anatase TiO_2, for which we are using the ABINIT code.

PAW Atomic Data Generation for ABINIT

M. Torrent and F. Jollet

Commissariat à l'Energie Atomique, Centre d'Etudes de Bruyères-le-Chatel, BP 12, F-91680 Bruyères-le-Chatel

Two PAW atomic data generators have been developed for ABINIT. The first one comes from the code ATOMPAW, written by N. Holzwarth and co-workers, that has been adapted for ABINIT. The second one comes from the ultrasoft generator from D. Vanderbilt. The presentation will include the following topics:

- Which data do we need?

- How are they generated?

- What is available on the web site?

- How to generate a new set of atomic data?

- How do the two generators compare?

Computation of non-linear optical properties from density functional perturbation theory

Marek Veithen[1], Philippe Ghosez[1], Xavier Gonze[2]

[1] *Département de Physique (B5), Université de Liège, Belgium*

[2] *Unité de Physico-Chimie et de Physique des Matériaux,*
Université Catholique de Louvain,
1 Place Croix du Sud, B-1348 Louvain-la-Neuve, Belgium

We present the recent implementation of third-order density functional perturbation theory in ABINIT in order to compute non-linear optical properties of periodic solids.

Following Nunes and Gonze [1], our approach makes use of the $2n + 1$ theorem applied to an electric field dependent energy functional. We first describe the general framework of the computation of third-order energy derivatives in ABINIT and their analysis with ANADDB.

Then, we focus on third-order energy derivatives with respect to three electric fields and two electric fields and one atomic displacement that are respectively related to the non-linear optical susceptibilities and the first-order change of the linear dielectric susceptibility induced by a cooperative atomic displacement. Combined with second-order energy derivatives such as the optical dielectric tensor, the Born effective charges and the interatomic force constants, these quantities allow to compute the Raman susceptibilities of transverse and longitudinal optical phonons and the electrooptic coefficients.

[1] R. W. Nunes and X. Gonze, Phys. Rev. B **63**, 155107 (2001).

First-principles study of periodic solids in a finite electric field

Marek Veithen[1], Philippe Ghosez[1], Karin Rabe[2], David Vanderbilt[2], Ivo Souza[3], and Jorge Íñiguez[4]

[1] *Département de Physique (B5), Université de Liège, Belgium*

[2] *Department of Physics and Astronomy, Rutgers University, New Jersey, USA*

[3] *Department of Physics, University of California, Berkeley, USA*

[4] *NIST Center for Neutron Research, National Institute of Standards and Technology,*
Maryland, USA

We present two methods for the first-principles calculation of insulators in a finite electric field and their implementation in the ABINIT code.

The first method allows to compute the structural response of a periodic insulating solid to a homogeneous static electric field within density functional perturbation theory (DFPT) [1]. We consider the thermodynamic potentials $E(\mathbf{R}, \eta, \boldsymbol{\mathcal{E}})$ and $F(\mathbf{R}, \eta, \mathbf{P})$, whose minimization with

respect to the internal structural parameters $\mathbf{R}$ and unit cell strain η yields the equilibrum structure at fixed electric field $\boldsymbol{\mathcal{E}}$ and polarization $\mathbf{P}$, respectively. A first-order expansion of $E(\mathbf{R}, \eta, \boldsymbol{\mathcal{E}})$ in $\boldsymbol{\mathcal{E}}$ leads to a useful approximation in which $\mathbf{R}(\mathbf{P})$ and $\eta(\mathbf{P})$ can be obtained by simply minimizing the zero-field internal energy with respect to structural coordinates subject to the constraint of a fixed spontaneous polarization $\mathbf{P}$.

The second technique consists in iteratively minimizing an electric field dependent energy functional [2] composed of the usual Kohn-Sahm energy E_{KS} and a field coupling term $-\Omega\mathbf{P} \cdot \boldsymbol{\mathcal{E}}$. E_{KS} and the polarization $\mathbf{P}$ are expressed in terms of a set of field-polarized Bloch functions. The functional has equivalent local minima below a critical field $\boldsymbol{\mathcal{E}}_c$ that depends inversely on the density of k points; the disappearance of the minima at $\boldsymbol{\mathcal{E}}_c$ signals the onset of Zener breakdown.

[1] N. Sai, K. M. Rabe and D. Vanderbilt, Phys. Rev. B **66**, 104108 (2002).

[2] I. Souza, J. Íñiguez and D. Vanderbilt, Phys. Rev. Lett. **89**, 117602 (2002).

The electron-phonon interaction in ABINIT

Matthieu Verstraete

Unité de Physico-Chimie et de Physique des Matériaux,
Université Catholique de Louvain,
1 Place Croix du Sud, B-1348 Louvain-la-Neuve, Belgium

The present state of the implementation of the electron-phonon coupling in ABINIT is presented. Basics of the theory and the structure of the present subroutines are overviewed. The steps users will have to go through to execute electron-phonon calculations are sketched out, and present conceptual problems are presented.

DOS and partial DOS in ABINIT: angular momentum projection and the tetrahedron method

Matthieu Verstraete

Unité de Physico-Chimie et de Physique des Matériaux,
Université Catholique de Louvain,
1 Place Croix du Sud, B-1348 Louvain-la-Neuve, Belgium

The traditional method for calculating the density of states has been supplemented by the tetrahedron method (TM) in ABINIT. The TM converges faster and gives better results by

interpolating the band structure and calculating the resulting contribution to the DOS. Pathological cases and caveats are presented. The projection of wavefunctions on angular momenta has also been implemented, and the output (contribution of s, p, d... to each band at each kpoint) is used to output projected DOS. Implementation and user inputs are discussed.

Experimentation with parareal molecular dynamics and Thomas-Fermi as a predictor

Aline Roy and Gilles Zerah

CEA/DAM, Ile de France, 91680 Bruyères-le-Chatel

We will present some experiments we performed using the parareal algorithm in the case of molecular dynamics of helium.

List of Participants

Secretary: Edmonde Le Du   `edmonde.ledu@cea.fr`

Douglas Allan   `allandc@corning.com`
Glass Research
Corning Incorporated
SP FR 5
14831 Corning NY (USA)

Bernard Amadon   `bernard.amadon@cea.fr`
Département de Physique Théorique et Appliquée
Commissariat à l'Énergie Atomique
BP 12
91680 Bruyères-le-Châtel (France)

Christophe Audouze   `christophe.audouze@math.u-psud.fr`
Laboratoire de Mathématique
Université Paris-Sud - Orsay
Bâtiment 425
91405 Orsay (France)

Jean-Michel Beuken   `beuken@pcpm.ucl.ac.be`
Unité PCPM
Université Catholique de Louvain
1 place Croix du Sud
1348 Louvain-la-Neuve (Belgium)

Silvana Botti   `silvana.botti@polytechnique.fr`
Laboratoire des Solides Irradiés
CNRS-CEA Ecole Polytechnique
Route de Saclay
91128 Palaiseau (France)

François Bottin   `francois.bottin@cea.fr`
Département de Physique Théorique et Appliquée
Commissariat à l'Énergie Atomique
BP 12

91680 Bruyères-le-Châtel (France)

Johann Bouchet   bouchet@pcpm.ucl.ac.be
Unité PCPM
Université Catholique de Louvain
1 place Croix du Sud
1348 Louvain-la-Neuve (Belgium)

Eric Bousquet   eric.bousquet@ulg.ac.be
Département de Physique
Université de Liège
Allée du 6 Août, 17
4000 Sart Tilman (Belgium)

Fabien Bruneval   fabien.bruneval@polytechnique.fr
Laboratoire des Solides Irradiés
CNRS-CEA Ecole Polytechnique
Route de Saclay
91128 Palaiseau (France)

Eric Cancès   cances@cermics.enpc.fr
Ecole Nationale des Ponts et Chaussés
Champs sur Marne
Cité Descartes
77745 Marne La Vallée (France)

Fabrizio Cleri   cleri@casaccia.enea.it
ENEA, Unità Materiali e Nuove Tecnologie
Centro Ricerche Casaccia
C.P. 2400
00100 Roma A.D. (Italy)

Michel Côté   michel.cote@umontreal.ca
Département de Physique
Université de Montréal
C.P. 6128, succ. Centre-ville
H3C 3J7 Montréal, Québec (Canada)

Muriel Delaveau   muriel.delaveau@cea.fr
Département de Physique Théorique et Appliquée
Commissariat à l'Énergie Atomique

BP 12
91680 Bruyères-le-Châtel (France)

Thierry Deutsch `tdeutsch@cea.fr`
DSM/DRFMC
CEA-Grenoble
17 avenue des Martyrs
38054 Grenoble Cedex 9 (France)

Fabio Finocchi `finocchi@gps.jussieu.fr`
Groupe Physique des Solides
CNRS
Campus de Boucicaut, 140 rue de Lourmel
75015 Paris (France)

Gregory Geneste `gregory.geneste@ulg.ac.be`
Département de Physique
Université de Liège
Allée du 6 Août, 17
4000 Sart Tilman (Belgium)

Philippe Ghosez `philippe.ghosez@ulg.ac.be`
Département de Physique
Université de Liège
Allée du 6 Août, 17
4000 Sart Tilman (Belgium)

Xavier Gonze `gonze@pcpm.ucl.ac.be`
Unité PCPM
Université Catholique de Louvain
Place Croix du Sud, 1
B-1348 Louvain-la-neuve (Belgium)

Donald Hamann `drh@bell-labs.com`
Physics Depatment
Bell Labs & Rutgers University
600 Mountain Ave.
07974 Murray Hill, NJ (USA)

François Jollet `francois.jollet@cea.fr`
Departement de Physique Théorique et Appliquée

Commissariat à l'Énergie Atomique
BP 12
91680 Bruyères-le-Châtel (France)

Jean-Paul Minet   minet@cism.ucl.ac.be

Institut de Calcul Intensif et de Stockage de Mass
Université Catholique de Louvain
Rue du Compas, 4
1348 Louvain-la-Neuve (Belgium)

Peter Murray-Rust   pm286@cam.ac.uk

Chemistry Department
University of Cambridge
Lensfield Road
CB2 1EW Cambridge (United Kingdom)

Gerald Jomard   gerald.jomard@cea.fr

Département de Physique Théorique et Appliquée
Commissariat à l'Énergie Atomique
BP 12
91680 Bruyères-le-Châtel (France)

Masayoshi Mikami   mikami.masayoshi@mv.m-kagaku.co.jp

Research and Technology Development Division
Mitsubishi Chemical Sci. & Tech. Research Center
1000, Kamoshida-cho, Aoba-ku Yokohama
227-8502 Yokohama (Japan)

Yann-Michel Niquet   yniquet@cea.fr

DRFMC/SP2M/L_Sim
CEA-Grenoble
17 avenue des Martyrs
38054 Grenoble Cedex 9 (France)

Spaldin Nicola   nicola@mrl.ucsb.edu

Materials Department
University of California
93106-5050 Santa Barbara, CA (USA)

Valerio Olevano   valerio.olevano@polytechnique.fr

Laboratoire des Solides Irradiés

CNRS-CEA Ecole Polytechnique
Route de Saclay
91128 Palaiseau (France)

Artem R. Oganov   `a.oganov@mat.ethz.ch`
Materials
ETH Zurich
5 Sonneggstrasse
CH-8092 Zurich (Switzerland)

Yann Pouillon   `pouillon@pcpm.ucl.ac.be`
Unité PCPM
Université Catholique de Louvain
1 place Croix du Sud
1348 Louvain-la-Neuve (Belgium)

Aline Roy   `aline.roy@cea.fr`
DSSI/SISR
Commissariat à l'Énergie Atomique
BP 12
91680 Bruyères-le-Châtel (France)

Vanina Recoules   `vanina.recoules@cea.fr`
Département de Physique Théorique et Appliquée
Commissariat à l'Énergie Atomique
BP 12
91680 Bruyères-le-Châtel (France)

Lucia Reining   `lucia.reining@polytechnique.fr`
Laboratoire des Solides Irradiés
CNRS-CEA Ecole Polytechnique
Route de Saclay
91128 Palaiseau (France)

Gian-Marco Rignanese   `rignanese@pcpm.ucl.ac.be`
Unité PCPM
Université Catholique de Louvain
1 place Croix du Sud
1348 Louvain-la-Neuve (Belgium)

Marc Torrent   marc.torrent@cea.fr

Département de Physique Théorique et Appliquée

Commissariat à l'Énergie Atomique

BP 12

91680 Bruyères-le-Châtel (France)

Florent Tournus   tournus@pcpm.ucl.ac.be

Unité PCPM

Université Catholique de Louvain

1 place Croix du Sud

1348 Louvain-la-Neuve (Belgium)

Marek Veithen   marek.veithen@ulg.ac.be

Département de Physique

Université de Liège

Allée du 6 aout 17

4000 Sart Tilman (Belgium)

Matthieu Verstraete   verstraete@pcpm.ucl.ac.be

Unité PCPM

Université Catholique de Louvain

1 place Croix du Sud

1348 Louvain-la-Neuve (Belgium)

Gilles Zerah   gilles.zerah@cea.fr

Département de Physique Théorique et Appliquée

Commissariat à l'Énergie Atomique

BP12

91680 Bruyères-le-Châtel (France)

5 News from UK's CCP9 Programme

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

5.1 Reports on CCP9 Workshops

5.1.1 Report on Hydrogen in Oxides Workshop

Hydrogen in Oxides

The Royal Institution, London, U.K.

Wednesday 21 April 2004

Organisers

Professor SFJ Cox

ISIS, Rutherford Appleton Laboratory and University College London
Dr DJ Keeble

University of Dundee

Dr A Shluger, University College London

Dr A Sokol

The Royal Institution of Great Britain

Sponsors

Materials and Characterisation Group of the Institute of Physics

EPSRC Network for Theory and Experiment in Extreme Nanotechnology

Collaborative Computational Projects CCP5 for Computer Simulation of Condensed Phases

CCP9 for Study of the Electronic Structure of Condensed Matter

This symposium and workshop brought together materials scientists, solid state and computational chemists, crystallographers and geologists, with a common interest in the title subject. It attracted 47 attendees and included participants from Italy, Portugal, Germany, Ireland, and the USA, as well as invited speakers from Belgium, Japan and Korea. The presentations included ten invited talks and a similar number of contributed posters, chiefly on aspects of structure and electrical activity. Discussions covered optical, electronic, and chemical applications, as well as mineralogical aspects. Abstracts of all the talks and posters may be found on the website of the ISIS Muon Group: www.isis.ac.uk/muons/hoxide.

The meeting was opened by M Welch (Natural History Museum) who introduced the importance of hydrogen in minerals, and of the significant reservoir of hydrogen within the Earth's mantle. These studies are at an early stage but the types of minerals and microscopic mechanisms of interest were seen to share common features with the studies of electronic materials and nano-porous chemical substrates.

JF Scott (Cambridge) reviewed the technological aspects of hydrogen in electronic oxides, particularly the perovskite oxides used in memory modules, and emphasised the current industrial relevance and importance. C-H Park (Pusan) described theoretical studies of hydrogen in these materials and provided insight on possible microscopic mechanisms for ferroelectric aging; he also discussed the possibly crucial role of hydrogen in dilute magnetic semiconducting oxides for spintronic applications. K Knight (ISIS) discussed the use of high-resolution neutron diffraction to study hydrogen sites in a perovskite oxides that exhibits protonic conduction. J Gavartin (UCL) provided theoretical insight on the dynamics of hydrogen in some of the materials under consideration as high-permittivity gate dielectrics and V Afanas'ev (Leuven) described experimental studies of charge trapping in these materials. H Hosono (Tokyo) described the central role played by hydrogen in the new transparent conducting oxide materials; P Sushko (UCL) described the theory of hydrogen in this class of materials.

One of the central topics of the meeting was the possibility of a universal model for the electrical activity of hydrogen in semiconductors and dielectrics. Theoretical and experimental studies provide evidence that hydrogen acts as a shallow donor, as a deep donor, or as an acceptor, depending on the band-edge positions. One school of theory proposes the existence of a universal pinning-level for hydrogen with a fixed relation to the vacuum level. J Robertson (Cambridge) gave a critique of this concept, as applied to complex oxides, and provided computational results at some variance with this model. SFJ Cox (ISIS) presented experimental results using muonium as a pseudo-isotope and accessible experimental model for hydrogen, reporting a number of new candidate shallow-donor states and providing an overview of the emerging systematics which was so far unavailable for hydrogen itself.

Given the topical importance of these issues and fast-moving developments in the field, a follow-up meeting concentrating on oxides as electronic materials was mooted.

6   General Workshop/Conference Announcements

6.1   The Third Conference of the Asian Consortium on Computational Materials Science (ACCMS3)

Autumn 2005, Beijing

We would like to bring to your attention that the ACCMS3 (The Third Conference of the Asian Consortium on Computational Materials Science) will be held in Autumn 2005 in Beijing.

Information on submitting abstracts will be posted in Autumn 2004.

Additional information on the conference can be found at

`http://www-lab.imr.edu/~accms/`

Please forward information on this conference to individuals who might benefit from participation.

Dr. Hiroshi Mizuseki
Institute for Materials Research
Tohoku University
URL: `http://www-lab.imr.edu/~mizuseki/contactme.html`

7 General Job Announcements

Postdoctoral Position

"Ab initio studies of alteration process at the surface of glasses"
Commissariat a l'Energie Atomique - France

A postdoctoral position for 12 months (with possible extention to 18 months) is opened in the Laboratoire du Comportement a Long Terme (LCLT) of CEA (Commissariat a l'Energie Atomique -France) in collaboration with the Modelisation Group of the Laboratoire des Verres (Univ. Montpellier 2, France).

The research will cover the study of the alteration processes at the surfaces of nuclear waste confinement glasses. The focus of the study will be the microscopic description of the solvation process by a combination of Ab initio and classical Molecular Dynamics simulations. Candidates must have a PhD in physics or theoretical chemistry and experience in Molecular Dynamics calculations.

Interested applicants should sent a Curriculum Vitae and statement of research to

Dr. Simona ISPAS,
email: simona.ispas@ldv.univ-montp2.fr
Laboratoire des Verres, cc 069
Universite Montpellier 2 Tel: +33 (0)4 67 14 49 79
34095 Montpellier Cedex 05 Fax: +33 (0)4 67 14 34 98,
FRANCE

Salary: 1940 Euro to 2097 Euro/month depending on qualifications .

Deadline: 1st of July 2004 or until the position is fulfilled.

Lecturer and Professor Positions
University of Bristol, U.K.

Bristol University is currently advertising the following three academic positions. See http://www.phy.bris.ac.uk/vacanies.htm for full details.

1. Professor of Physics and Head of the Department of Physics (ref. 10272)

The University of Bristol seeks to appoint an individual of the highest international calibre to a Chair in Physics. The successful applicant will be expected to lead the development of Physics as Head of the Department on appointment.

The successful applicant will be involved in making six new academic posts in Physics over the next two years in fulfilment of the University plan for the Department. The University is constructing a state-of-the-art building specially designed for interdisciplinary research in nanoscience and quantum information immediately adjacent to the Physics building, and is also committed to refurbishment of the Department's teaching and research facilities.

This is a major opportunity to shape one of the UK's leading Departments of Physics, and the University expects the successful applicant to have outstanding qualities of academic leadership and intellectual vision appropriate to achieving and maintaining a department of the highest international reputation.

2. Lecturer in Theoretical Physics (ref. 10327)

The Department of Physics seeks to appoint a Lecturer in Theoretical Physics, with effect from 1 November 2004 or as soon as possible thereafter. The successful applicant will have an outstanding research record in an area which complements and enhances our current research activities in theoretical physics. These lie in condensed matter theory and nanoscience, in quantum information and in geometric aspects of waves; for more information see

http://www.phy.bris.ac.uk/research/theory/home.html

3. Lecturer in Experimental Condensed Matter Physics (ref. 10328)

The Department of Physics seeks to appoint a Lecturer in Experimental Condensed Matter Physics, with effect from 1 November 2004 or as soon as possible thereafter. Preference will be given to applicants whose research activities complement and enhance existing activities of the condensed matter physics group. These currently centre on the physics of strongly-correlated electron systems and include superconductivity, quantum magnetism and electronic structure. The group has extensive in-house facilities for the preparation and characterisation

of novel electronic materials. These include a suite of high-field and low temperature facilities, and positron annihilation spectroscopy facilities. The group's current research programmes are available at

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http://www.phy.bris.ac.uk/research/cond_matt/home.html
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Post-doctoral Position in Condensed Matter Theory

Department of Physics, Kaiserslautern University of Technology, Germany

The Condensed Matter Theory Group (AG Hübner) at the Department of Physics, Kaiserslautern University of Technology, Germany, invites applications for a post-doctoral position within the EU research training network EXCITING.

The successful candidate is expected to carry out research within the topic "Ab-initio calculations of static and dynamic excited-state properties of metal nanoparticles". Candidates must have completed a Ph.D. in a topic relevant to the position, be less than 35 years of age, be citizens of an EU country other than Germany, and have spent less than 12 months in Germany within the 24 months prior to the appointment date. Salary will be according to the German BAT IIa scale.

The position is available initially for 12 months, with the possibility of extension. The position is available immediately, and search for a suitable candidate will proceed until the position is filled.

Women and disbled persons are encouraged to apply.

Applications should include a CV, a list of publications, a list of three references, and should be directed to Dr. Torsten Andersen (thor@physik.uni-kl.de) or Prof. Dr. Wolfgang Hübner (huebner@physik.uni-kl.de), Department of Physics, Kaiserslautern University of Technology, Box 3049, D-67653 Kaiserslautern, Germany.

E-mail applications are accepted in plain text or PDF only.

Chair and Lectureship in Atomistic Simulation

Atomistic Simulation Centre,
Queen's University, Belfast, U. K.
Reference numbers: 04/L062A and 04/K410A

The Atomistic Simulation Centre (ASC) (formerly the Atomistic Simulation Group) invites applications for newly created posts of Professor and Lecturer in Atomistic Simulation in the School of Mathematics and Physics, Queen's University Belfast, tenable from 1 October 2004. The ASC, led by Professor Mike Finnis, embraces the Theory and Simulation of Liquids and Solids Research Division in the School of Mathematics and Physics and Dr. Peijun Hu's catalysis research group in the School of Chemistry.

The interests of the current five permanent members of staff are broad, as indicated on the web pages

http://titus.phy.qub.ac.uk.

With the new posts we particularly seek to increase our strength in statistical mechanical methods, electronic structure (beyond standard density functional methods and including time dependent problems) and the structure and function of biological molecules.

We are seeking outstanding scientists with a track record of internationally recognised research, commensurate years of experience, working in one or more of the following fields: innovative simulation based on electronic structure (i.e. going beyond standard applications of density functional theory); statistical mechanics applied to atomistic simulation; insightful simulation of systems of biological relevance.

The appointee will be expected to take part in the teaching of applied mathematics and theoretical physics to undergraduate students at all levels of these subjects, and to share in the usual administrative duties of academic staff.

Applications should be made on the forms obtainable from

http://www.qub.ac.uk/jobs/

as follows.

On that webpage enter the job type as 'ACADEMIC' and scroll to the post you are interested in, where you can complete and download the application form together with further particulars of the posts.

Closing dates for applications:

Chair: 6 August 2004; Lectureship: 23 July 2004

Informal enquiries may be directed to Dr. Tchavdar Todorov (t.todorov@qub.ac.uk) or Dr. Jorge Kohanoff (j.kohanoff@qub.ac.uk).

Semiconductor Physics Postdoc

National Renewable Energy Laboratory
Golden, Colorado

We invite applications for a postdoctoral researcher in Computational Sciences Center at the National Renewable Energy Lab. The successful candidate will work closely with physicists, computational scientists, and mathematicians to develop new mathematical and computational methodologies capable of designing materials with relevant properties using electronic structure methods for million atom nanostructures. Significant use of supercomputing resources is expected.

Applicants need to have a PhD in physics, material science, chemistry, or related field. Demonstrated experience in research and development in electronic structure methods for semiconductors is preferred. Interest in algorithmic/mathematical development and scientific programming ability, including parallel programming, is desired. For detailed information on this position see

`http://www.nrel.gov/hr/employment/rpp/jobs_files/5174.html`.

NREL is the U.S. Dept. of Energy's premier laboratory for renewable energy and energy efficiency and we are located just south of Boulder and west of Denver. More information on the research activities at NREL can be found at

http://www.nrel.gov.

Please submit your resume and cover letter by mail, fax, or email, to: Beverly Maestas (`REQ# 5300-5174`), NREL, 1617 Cole Blvd., Golden, CO 80401, Fax: 303/384-7599, or `beverly_maestas@nrel.gov` (A. A. / E. O. E.)

Kwiseon Kim, Ph.D. Computational Sciences Center National Renewable Energy Laboratory 1617 Cole Blvd. Mail Stop 1608 Golden, CO 80401

`kwiseon_kim@nrel.gov` phone: (303)275-4122 fax: (303)275-4007

PhD Scholarship and Postdoctoral Position

in "Atomistic Simulations of Metallic Glasses"

Center for Atomic-scale Materials Physics (CAMP)

Department of Physics

Technical University of Denmark (DTU)

Bulk metallic glasses (BMGs) are fascinating new materials with extraordinary mechanical properties. A newly formed European research and training network (RTN) focuses on the development of ductile high-strength BMG composites, and in this connection we invite applications for a PhD scholarship and a postdoctoral position to work on the mechanical properties of metallic glasses using atomistic computer simulations. The research is to be conducted at the Center for Atomic-scale Materials Physics (CAMP) at the Department of Physics, the Technical University of Denmark (DTU) and is expected to be carried out in close collaboration with the other partners of the RTN.

Postdoctoral position:

Candidates for the postdoctoral position should have a PhD in physics or materials science with experience in atomistic computer simulations and/or electronic structure calculations. The appointment will be initially for one year with possible extension to two years. The salary and appointment terms are consistent with the current collective agreement for Danish Universities. The monthly salary is approximately Euro 3300.

Applications including curriculum vitae, list of publications, and the names, affiliations, and e-mail addresses of three references should be sent as soon as possible preferably in electronic form to the address below.

PhD scholarship:

Candidates for the PhD scholarship should have a master's degree in condensed matter physics, engineering physics, or equivalent. The scholarship is for three years leading to a PhD degree from the Technical University of Denmark. The salary and appointment terms are consistent with the current DTU rules for PhD degree students. The scholarship is co-financed by the RTN, the Copenhagen Graduate School for Nanoscience and Nanotechnology, and DTU. The monthly salary is approximately Euro 2800. Applications including curriculum vitae and the names, affiliations, and e-mail addresses of two references should be sent as soon as possible preferably in electronic form to the address below.

More information on the positions can be obtained from Professor Karsten W. Jacobsen at kwj@fysik.dtu.dk or from Associate Professor Jakob Schiotz at schiotz@fysik.dtu.dk.

Information on CAMP can be found at http://www.fysik.dtu.dk/ and information on the RTN "Ductile BMG Composites" can be found at http://www.inpg.fr/BMG-RTN/.

Because the funding is from an RTN, preference will be given to non-Danish candidates from European countries.

Applications should be sent to:

Professor Karsten W. Jacobsen,
CAMP, Department of Physics
Technical University of Denmark, Building 307
DK-2800 Kongens Lyngby, Denmark
E-mail: kwj@fysik.dtu.dk

Post-Doc Opening in "Theory of Carbon Nanotube Electronics" Institute of Applied Physics of the University of Hamburg, Germany

A post-doc position is available at a recently established research group for theory of magneto- and nanoelectronics at the Institute of Applied Physics of the University of Hamburg. The focus of our group is the exploration of physical properties and processes of new materials for applications in nano- and spinelectronics based on electronic structure calculations with different degrees of complexity. Collaborations with experimental groups at the institute and theory groups at the Forschungs- zentrum Juelich have been established in the past.

In particular we are looking for a candidate to work in the field of carbon nanotube based electronics. Using a combination of ab-initio and tight-binding calculations we want to explore transport properties of novel devices. An existing tight-binding code for the calculation of non-equilibrium transport in carbon nanotube devices should be extended for a better inclusion of the electronic structure of the contacts. In particular we want to treat the coupling to magnetic electrodes to study spin-transport in such devices.

Applicants need to have a PhD in physics, material science, chemistry, electrical engineering or related fields. Applicants who demonstrate experience in computer simulations in condensed matter physics in particular in electronic structure calculations (semi-empirical or ab-initio) are preferred.

The Institute of Applied Physics of the University of Hamburg is one of the top laboratories for nanocience in Germany. A focus of the Institute are transport in low-dimensional structures and magnetism of nanostructures (e.g. http://www.nanoscience.de).

The lab is located downtown in Hamburg, one of the most attractive cities in Germany, with a great nightlife, a lot of opportunities for outdoor activities, a high quality of life, and many cultural events.

More information on the research activities at the Institute of Applied Physics of the University of Hamburg can be found at
http://www.physnet.uni-hamburg.de/institute/IAP/angew.html

The position starts September 1, 2004 and ends August 31, 2006, with a possible extension of one year. The salary is according to BAT IIa which is about 40.000 Euros per year.

Please submit your inquiries or your resume and cover letter by mail, fax, or email, to:

Dr. Stefan Heinze,
Institute of Applied Physics, University of Hamburg,
Jungiusstrasse 9a, 20355 Hamburg,
Germany
Fax: +49-40-42838-5311
Email: heinze@physnet.uni-hamburg.de
Internet: http://www.nanoscience.de/stefan

Research Associate

Developing Multiscale Techniques to Connect the Quantum to the Mesoscopic Level

Theoretical Chemistry, Ruhr-Universitaet Bochum, Germany

Applications are invited for a research associate position.

Subject to funding the preferred starting date would be fall/winter 2004.

The ideal candiate would have significant experience in electronic structure theory, mixed quantum/classical simulation, and dynamical multiscale simulation. She or he would work primarily on developing and implementing novel techniques to connect a quantum description (Car-Parrinello) via a microscopic level to a coarse-grain treatment. Although the ultimate goal is to predict properties of soft materials, the project focuses heavily on code development in close collaboration with an outstanding partner group. In addition, he/she can also be involved in other challenging research projects including both method development and large-scale applications.

Information on the techniques used and developed are accessible via

http://www.theochem.rub.de/go/cprev.html.

The Center of Theoretical Chemistry at RUB offers an exciting interdisciplinary environment with excellent working conditions (including several parallel platforms and a 500 GFlop/s SCI machine in house).

Candidates should send a detailed resume including an outline of their research achievements and interests as well as contact information for academic references as one pdf file to office@theochem.rub.de.

Consideration of candidates will begin immediately and continue until the position is filled. The University particularly welcomes applications from women.

Dominik Marx
Lehrstuhl fuer Theoretische Chemie
Ruhr-Universitaet Bochum
44780 Bochum, Germany
Email: office@theochem.rub.de
Fax: ++49 234 32 14045
URL: http://www.theochem.rub.de/

8 Abstracts

Magnetic moments of ferromagnetic, superparamagnetic, and submonolayer Fe on a GaAs(100) surface

J. S. Claydon and Y. B. Xu

Department of Electronics, Spintronics Laboratory,
The University of York, York YO10 5DD, United Kingdom

M. Tselepi and J. A. C. Bland

Cavendish Laboratory, University of Cambridge,
Cambridge CB3 0HE, United Kingdom

G. van der Laan

Magnetic Spectroscopy, Daresbury Laboratory,
Warrington WA4 4AD, United Kingdom

Abstract

We have used x-ray magnetic circular dichroism (XMCD) to determine the spin and orbital magnetic moments of Fe atoms at the ferromagnetic/superparamagnetic boundary, superparamagnetic thickness, and submonolayer thickness at the interface. The samples, grown by molecular beam epitaxy at room temperature, were 5, 4, and 0.5 ML (monolayer) Fe on GaAs (100)-4×6 capped with 7 ML Cr, preceded in the case of the 0.5 ML Fe by 9 ML Co. The XMCD results show orbital moments enhanced by almost 300% with respect to the bulk and bulklike spin moments for all three thicknesses demonstrating unambiguously that the Fe/GaAs interface is magnetic.

Orientation Effects in the Electronic and Optical Properties of Germanium Quantum Wires

A. N. Kholod[1], V. L. Shaposhnikov[2,3], N. Sobolev[2] V. E. Borisenko[3],

F. Arnaud D'Avitaya[4], and Stefano Ossicini[5]

[1] *Federal Office of Communications, P. O. Box,*
2501 Biel-Bienne, Switzerland

[2] *Department of Physics, University of Aveiro, 3810-193 Aveiro, Portugal*

[3] *Belarusian State University of Informatics and Radioelectronics,*
P. Browka 6, 220027 Minsk, Belarus

[4] *Centre de Recherche sur les Mécanismes de la Croissance Cristalline,*
CNRS, Campus de Luminy, Case 913, 13288, Marseille Cedex 9, France

[5] *INFM-S³ "nanoStructures and bioSystems at Surfaces" and*
Dipartimento di Scienze e Metodi dell'Ingegneria, Università di Modena
e Reggio Emilia, via Allegri 13, I-42100 Reggio Emilia, Italy

Abstract

We have performed first principles calculations in order to analyze the influence of spatial orientation on the electronic band structure and optical properties of hydrogenated germanium quantum wires. A quantum confinement induced direct band gap appears for the (110)-oriented wires, whereas the (100)- and (111)-oriented wires are characterized by an indirect band gap. For the same wire effective size an anisotropy in the fundamental band gap E_g with respect to the wire orientation is observed. For (110)-oriented wires the imaginary part of the dielectric function shows a pronounced peak in the visible energy range with strong dimensionality and polarization dependence.

Contact person: ossicini@unimore.it

Magnetic properties of stoichiometric and nonstoichiometric ultrathin Fe_3O_4(111) films on Al_2O_3(0001)

F. Schedin and E. W. Hill

Centre for Mesoscience and Nanotechnology
and Department of Computer Science,
University of Manchester, Manchester M13 9PL, United Kingdom

G. van der Laan

Magnetic Spectroscopy, Daresbury Laboratory,
Warrington WA4 4AD, United Kingdom

G. Thornton

Department of Chemistry, University of Manchester,
Manchester M13 9PL, United Kingdom

Abstract

A detailed characterization of magnetic oxide films is essential to enable their use in magnetoresistive devices since their properties depend critically on stoichiometry and structural order. Here, the composition and magnetic properties of ultrathin iron oxide films grown epitaxially on Al_2O_3(0001) have been characterized using x-ray magnetic circular dichroism (XMCD) and magnetoresistance (MR) measurements. The XMCD data show by comparison with theoretical calculations that we have successfully found growth conditions for well ordered epitaxial films with Fe_3O_4 stoichiometry. Nonstoichiometric films exhibit, in addition to a relative reduction in Fe^{2+} ions, a net transfer of Fe^{3+} from tetrahedral to octahedral sites. The in-plane MR for both these films is found to be 1% at room temperature in a field of 1 T even though the electrical conductivity differs by a factor of 5.

Self-interaction correction in multiple scattering theory

M. Lüders[1], A. Ernst[2], M. Däne[3,1], Z. Szotek[1], A. Svane[4], D. Ködderitzsch[3,1],
W. Hergert[3], B. L. Györffy[5], and W. M. Temmerman[1]

[1] *Daresbury Laboratory, Daresbury, Warrington, WA4 4AD, UK*
[2] *Max Planck Institut für Mikrostrukturphysik,*
Weinberg 2, D-06120 Halle, Germany
[3] *Martin-Luther-Universität Halle-Wittenberg,*
Friedemann-Bach-Platz 6, D-06099 Halle, Germany
[4] *Institute of Physics and Astronomy, University of Aarhus,*
DK-8000 Aarhus, Denmark
[5] *H.H. Wills Physics Laboratory, University of Bristol,*
Tyndall Avenue, Bristol BS8 1TL, UK

Abstract

We propose a simplified version of self-interaction corrected local spin-density (SIC-LSD) approximation, based on multiple scattering theory, which implements self-interaction correction locally, within the KKR method. The multiple scattering aspect of this new SIC-LSD method allows for a straightforward generalisation to the coherent potential approximation (CPA). This facilitates applications of the SIC to alloys and pseudoalloys which could describe disordered local moment systems, as well as intermediate valences. This new method is a first step towards a dynamical SIC, a method which will allow for dynamical valence and spin fluctuations. As a demonstration of the method, we study the well-known α-γ phase transition in Ce, where we also explain how SIC operates in terms of multiple scattering theory.

A step up to self-assembly

Kristen Fichtorn[1] and Matthias Scheffler[2]

[1]*Pennsylvania State University, Pennsylvania 16802, USA*

[2]*Fritz-Haber-Institut der Max-Plank-Gesellschaft, Faradayweg 4–6,
D-14195 Berlin-Dahlem, Germany*

Abstract

Powerful computer simulations have resolved the mechanism for the nanoscale assembly of the 'hut'-like clusters that form after a few layers of atoms have been deposited on certain solid surfaces.

The steady-state of heterogeneous catalysis, studied by first-principles statistical mechanics

Karsten Reuter[1,2], Daan Frenkel[2] and Matthias Scheffler[1]

[1]*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6,
D-14195, Berlin, Germany*

[2]*FOM Institute for Atomic and Molecular Physics, Kruislaan 407,
SJ1098 Amsterdam, The Netherlands*

Abstract

The turn-over frequency of the catalytic oxidation of CO at $RuO_2(110)$ was calculated as function of temperature and partial pressures using *ab initio* statistical mechanics. The underlying energetics of the gas-phase molecules, dissociation, adsorption, surface diffusion, surface chemical reactions, and desorption were obtained by all-electron density-functional theory. The resulting CO_2 formation rate [in the full (T, p_{CO}, p_{O_2})-space], the movies displaying the atomic motion and reactions over times scales from picoseconds to seconds, and the statistical analyses provide insights into the concerted actions ruling heterogeneous catalysis and open thermodynamic systems in general.

Electronic Structure of Samarium Monopnictides and Monochalcogenides

A. Svane[1], V. Kanchana[2], G. Vaitheeswaran[2], G. Santi[1],

W. M. Temmerman[3], Z. Szotek[3], P. Strange[4] and L. Petit[1,5]

[1] *Department of Physics and Astronomy, University of Aarhus,*

DK-8000 Aarhus C, Denmark

[2] *Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany*

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

[4] *Department of Physics, Keele University, ST5 5DY, UK*

[5] *Computer Science and Mathematics Division, and Center for Computational Sciences,*

Oak Ridge National Laboratory,

Oak Ridge, Tennessee 37831-6114, USA

Abstract

The electronic structures of SmX (X=N, P, As, Sb, Bi, O, S, Se, Te, Po) compounds are calculated using the self-interaction corrected local-spin density approximation. The Sm ion is described with either five or six localized f-electrons while the remaining electrons form bands, and the total energies of these scenarios are compared. With five localized f-electrons a narrow f-band is formed in the vicinity of the Fermi level leading to an effective intermediate valence. This scenario is the ground state of all the pnictides as well as SmO. With six localized f-electrons, the chalcogenides are semiconductors, which is the ground state of SmS, SmSe and SmTe. Under compression the Sm chalcogenides undergo first order transitions with destabilization of the f states into the intermediate valence state, the bonding properties of which are well reproduced by the present theory.

Residual resistivity of diluted III-V magnetic semiconductors

I. Turek[1,2,3], J. Kudrnovský[3,4], V. Drchal[3,4] and P. Weinberger[3]

[1] *Institute of Physics of Materials, ASCR,*
Brno, Czech Republic

[2] *Department of Electronic Structures, Charles University in Prague,*
Czech Republic

[3] *Center for Computational Materials Science, TU Vienna, Austria*

[4] *Institute of Physics, ASCR, Prague, Czech Republic*

Abstract

The electronic structure and residual resistivity of diluted (Ga,Mn)As magnetic semiconductors are calculated from first principles using the linear muffin-tin orbital method, the coherent potential approximation, and the Kubo-Greenwood linear response theory. Particular attention is paid to the role of native compensating defects such as As antisites and Mn interstitials as well as to different magnetic configurations of the local Mn moments. The order of magnitude of the calculated resistivities compares reasonably well with available experimental data. The concentration variations of the resistivity reflect two basic mechanisms, namely the strength of the 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.

Calculations on different length scales for improving Processing of Nano-Ceramics

Wilfried Wunderlich

Nagoya Institute of Technology, Dept. of Environmental Technology,
Gokiso, Showa-ku, 466-8555 Nagoya, Japan

Abstract

Advanced processing of nano-ceramic composite materials requires an understanding of physical phenomena on an atomistic scale by ab-initio calculations. This overview continues a previous report and is divided into three parts. After describing the goals and the range of possible applications of such simulations, the needs for simulations of new applications of ceramics, namely for photovoltaic and thermoelectric materials, are briefly summarized. The most challenging subject for ab-initio calculations, however, is an understanding of physical phenomena in aqueous solutions and their present results are described in the third part. Based on experimental results, the simulation of Al-Mg-spinel formation with different methods, the discrete element method (DEM) and Molecular Dynamics (MD) is described. The appropriate approach for the numerical treatment of these many-particle interactions in liquids is the Voronoi- method, for which some new ideas are presented in this paper. For ab-initio calculations the software Vasp with its great facilities is appropriate.

Screening of Coulomb interactions in transition metals

I. V. Solovyev and M. Imada

Institute for Solid State Physics, University of Tokyo,

Kashiwanoha 5-1-5, Kashiwa, Chiba 277-8531, Japan

and

PRESTO, Japan Science and Technology Agency

Abstract

We discuss different methods of calculation of the screened Coulomb interaction U in transition metals and compare the so-called constraint local-density approximation (LDA) with the GW approach. We clarify that they offer complementary methods of treating the screening and, therefore, should serve for different purposes. In the *ab initio* GW method, the renormalization of *bare* on-site Coulomb interactions between $3d$ electrons (being of the order of 20-30 eV) occurs mainly through the screening by the same $3d$ electrons, treated in the random phase approximation (RPA). The basic difference of the constraint-LDA method from the GW method is that it deals with the neutral processes, where the Coulomb interactions are additionally screened by the "excited" electron, since it *continues to stay in the system*. This is the main channel of screening by the itinerant ($4sp$) electrons, which is especially strong in the case of transition metals and missing in the GW approach, although the details of this screening may be affected by additional approximations, which typically supplement these two methods. The major drawback of the conventional constraint-LDA method is that it does not allow to treat the energy-dependence of U, while the full GW calculations require heavy computations. We propose a promising approximation based on the combination of these two methods. First, we take into account the screening of Coulomb interactions in the $3d$-electron-line bands located near the Fermi level by the states from the subspace being orthogonal to these bands, using the constraint-LDA methods. The obtained interactions are further renormalized within the bands near the Fermi level in RPA. This allows the energy-dependent screening by electrons near the Fermi level including the same $3d$ electrons.

Intrinsic point defects and volume swelling in ZrSiO$_4$ under irradiation

J.M. Pruneda, T. D. Archer and Emilio Artacho

Department of Earth Sciences, University of Cambridge,
Downing Street, Cambridge, CB2 3EQ, United Kingdom

Abstract

The effects of high concentration of point defects in crystalline ZrSiO$_4$ as originated by exposure to radiation, have been simulated using first principles density functional calculations. Structural relaxation and vibrational studies were performed for a catalogue of intrinsic point defects, with different charge states and concentrations. The experimental evidence of a large anisotropic volume swelling in natural and artificially irradiated samples is used to select the subset of defects that give similar lattice swelling for the concentrations studied, namely interstitials of O and Si, and the anti-site Zr$_{Si}$. Calculated vibrational spectra for the interstitials show additional evidence for the presence of high concentrations of some of these defects in irradiated zircon.

Lattice dynamics of sodium alanate phases by a first-principles study

Xuezhi Ke

Fukui Institute for Fundamental Chemistry, Kyoto University,

Kyoto 606-8103, Japan

Isao Tanaka

Department of Materials Science and Engineering, Kyoto University,

Sakyo, Kyoto 606-8501, Japan

Abstract

The electronic properties and lattice dynamics of the sodium alanate phases have been studied by the density functional calculations. The phases include $NaAlH_4$ (space group: $I4_1/a$), Na_3AlH_6 (space group: $P2_1/n$), and NaH (space group: $Fm\text{-}3m$). The electronic properties are discussed on the basis of the electronic band structures, the atomic charges, the bond overlap population analysis, and the Born effective charges. The phonon dispersion relations and phonon density of states (DOS) of the phases are calculated by a direct force-constant method. Based on the integrated phonon DOS, the calculated thermodynamic functions including the heat capacity, the vibrational enthalpy, and the vibrational entropy are in good agreement with experimental values. Three decomposition reactions are studied based on the thermodynamic functions. The reactions are (1) $NaAlH_4 \rightarrow \frac{1}{3}Na_3AlH_6 + \frac{2}{3}Al + H_2$, (2) $\frac{1}{3}Na_3AlH_6 \rightarrow NaH + \frac{1}{3}Al + \frac{1}{2}H_2$, and (3) $NaH \rightarrow Na + \frac{1}{2}H_2$. The reactions (1), (2), and (3) are predicted to take place at 305, 400, and 726 K, respectively, which are in good agreement with the experiment (353, 423, and 698 K, respectively). The individual contributions to the reactions including the enthalpy and entropy are investigated. Concerning the entropy contribution ($T\Delta S$ term) to the reactions, we found that the net entropy contribution to the reaction is approximately equal to the entropy contribution from the H_2 gas molecule (produced in that reaction).

The influence of electronic structure on hydrogen absorption in palladium alloys

Xuezhi Ke and Gert Jan Kramer

Schuit Institute of Catalysis, Eindhoven University of Technology,

P.O. Box 513, 5600 MB Eindhoven, The Netherlands

Ole Martin Løvvik

Department of Physics, University of Oslo,

P.O.Box 1048 Blindern, N-0316 Oslo, Norway

Abstract

The influence of the electronic structure and of the lattice constant on hydrogen absorption in bulk Pd_3M_1 (M = Cd, Ag, Au, Pd, Cu, Ni, Pt, Pb, Sn, Fe, Rh, and Ru) has been studied by density functional calculations. We have assumed face-centered cubic structure of all the alloys, and hydrogen has been placed in the octahedral site surrounded by six Pd atoms. We have calculated the absorption energy of hydrogen in the alloys, and found that the influence of the electronic structure is much more important than that of the lattice constant. The results demonstrate that the Miedema's empirical rule is satisfied also in this system, that is the higher the binding energy of the host alloy, the less stable the hydride. We have also calculated the detailed electronic structure of the alloys and their hydrides. We found that more stable hydrogen absorption is correlated with the hydrogen $1s$-electrons, the palladium s electrons, the palladium s-like electrons, and the palladium d-electrons moving higher in the energy, towards the Fermi level. The two latter relations have previously been described for bulk systems and surfaces, respectively, while this study is apparently the first to point out the correlation between the position of the hydrogen band and the stability of hydride, i.e., the deeper the hydrogen band, the less stable the hydride.

Exotic Kondo effect from magnetic trimers

B. Lazarovits[1], P. Simon[2], G. Zaránd[3], and L. Szunyogh[1,3]

[1] *Center for Computational Materials Science, Vienna University of Technology,*
Gumpendorferstr. 1.a., A-1060 Vienna, Austria
[2] *Laboratoire de Physique et Modélisation des Milieux Condensés,*
CNRS et Université Joseph Fourier, 38042 Grenoble, France
[3] *Department of Theoretical Physics, Center for Applied Mathematics and*
Computational Physics, Budapest University of Technology and Economics,
Budafoki út 8., H-1521 Budapest, Hungary

Abstract

Motivated by the recent experiments of Jamneala *et al.* [T. Jamnaela *et al.*, Phys. Rev. Lett. **87**, 256804 (2001)], by combining *ab-initio* and renormalization group methods, we study the strongly correlated state of a Cr trimer deposited on gold. Internal orbital fluctuations of the trimer lead to huge increase of T_K compared to the single ion Kondo temperature explaining the experimental observation of a zero-bias anomaly for the trimers. The strongly correlated state seems to belong to a new, yet hardly explored class of non–Fermi liquid fixed points.

Manuscript available at `cond-mat/0407399`

Magnetic properties of Quantum Corrals from 'first principles' calculations

B. Lazarovits[1], B. Újfalussy[2], L. Szunyogh[1,3], B. L. Györffy[1,4], and P. Weinberger[1]

[1] *Center for Computational Materials Science, Vienna University of Technology, Gumpendorferstr. 1.a., A-1060 Vienna, Austria*

[2] *Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*

[3] *Department of Theoretical Physics, Center for Applied Mathematics and Computational Physics, Budapest University of Technology and Economics, Budafoki út 8., H-1521 Budapest, Hungary*

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

Abstract

We present calculations for electronic and magnetic properties of surface states confined by a circular quantum corral built of magnetic adatoms (Fe) on a Cu(111) surface. We show the oscillations of charge and magnetization densities and the possibility of the appearance of spin-polarized states. In order to classify the peaks in the calculated density of states with orbital quantum numbers we analyzed the problem in terms of a simple quantum mechanical circular well model. This model is also used to an estimate the behavior of the magnetization and energy with respect to the radius of the circular corral. The calculations are performed fully relativistically using the embedding technique within the Korringa-Kohn-Rostoker method.

Direct Observation of a Bulklike Spin Moment at the Fe/GaAs(100)-4×6 Interface

J. S. Claydon and Y. B. Xu

Spintronics Laboratory, Department of Electronics, The University of York, UK

M. Tselepi and J. A. C. Bland

Cavendish Laboratory, University of Cambridge, UK

G. van der Laan

Daresbury Laboratory, Warrington, WA4 4AD, UK

Abstract

We have used x-ray magnetic circular dichroism, which offers a unique capability to give element specific information at submonolayer sensitivity, to determine the spin and orbital magnetic moments at the Fe/GaAs(100) interface. The wedge samples, grown by molecular beam epitaxy at room temperature, consisted of 0.25-1 monolayer (ML) Fe on GaAs(100)-4×6 capped with 9 ML Co and have shown Fe spin moments of 1.84-1.96 μ_B and a large orbital enhancement. Our results demonstrate unambiguously that the Fe/GaAs(100)-4×6 interface is ferromagnetic with a bulklike spin moment, which is highly promising for spintronics applications.

9   SCIENTIFIC HIGHLIGHT OF THE MONTH

Partial dislocations in wurtzite GaN

J. Kioseoglou, G. P. Dimitrakopulos, Ph. Komninou, H. M. Polatoglou, and Th. Karakostas

Department of Physics, Aristotle University of Thessaloniki, GR-54124 Thessaloniki, Greece

Abstract

The atomic structures and energies of $1/6 < 20\bar{2}3 >$ and $1/3 < 10\bar{1}0 >$ partial dislocations in wurtzite GaN are modelled using an empirical interatomic potential in combination with topological theory and anisotropic elasticity calculations. Twelve stable configurations of the $1/6 < 20\bar{2}3 >$ edge and mixed partial dislocations that bound I_1 intrinsic basal stacking faults are obtained for each polarity and their core radii, energies, and atomic configurations are given. Moreover, the $1/3 < 10\bar{1}0 >$ edge and mixed partial dislocations along the junction lines between inversion domain boundaries (IDBs) and I_1 stacking faults are studied. Twenty eight stable junction line configurations have been identified, sixteen of them resulting in stable transformations of the energetically favourable IDB* defect to the electrically active Holt type IDB. The majority of the dislocation core structures possessed either dangling bonds or highly strained bonds. Since reduced coordination or strained bonds can introduce gap states, such dislocations could be electrically active.

1. Introduction

The influence of dislocations on the electrical, optical and mechanical properties of Ga-based III-nitride semiconductors is currently under intense investigation. Efficient optical devices such as blue-light-emitting diodes are commercially available despite the presence of a high density ($\sim 10^9$ cm^{-2}) of threading dislocations [1]. Theoretical and experimental investigations so far have concentrated on lattice dislocations. Initial theoretical results using *ab initio* calculations

indicated that charge-neutral edge and screw threading dislocations do not contribute to gap states and they are electrical inactive [2]. This has been disputed by other *ab initio* studies which have shown that edge dislocations may be charged, giving rise to deep-gap states [3], [4]. Dependence of the core formation energies on the Fermi level and growth stoichiometry has also been examined [3]. Moreover tight binding calculations have shown evidence for empty gap states associated with edge dislocations in the top half of the gap [5]. Also, by the use of first-principles calculations of electron energy-loss spectra, has been shown gap stage associated with edge dislocations [6]. Regarding the screw dislocations, full core structure has been observed using Z-contrast imaging [7] and the open core structure by transmission electron microscopy, [8] [9] while their electrical activity has been related to the growth stoichiometry [10]. More recently new structures for the screw dislocation have been proposed under certain growth conditions [11] [12].

Beside the perfect lattice dislocations, optoelectronic properties of devices should be also influenced by the partial dislocations when they exist in large numbers. The aim of the present contribution is to perform a systematic investigation of the core structures and the corresponding energies of the $1/6 < 20\bar{2}3 >$ edge and mixed partial dislocations that bound I_1 intrinsic basal stacking faults in wurtzite GaN, and of the $1/3 < 10\bar{1}0 >$ edge and mixed partial dislocations along the junction lines between inversion domain boundaries (IDBs) and I_1 stacking faults (SFs). Core radii and energies are evaluated in an approach combining anisotropic elasticity, topological theory and atomistic calculations. Initially, the dislocation displacement field of the $1/6 < 20\bar{2}3 >$ edge and mixed partial dislocations is imposed according to anisotropic elasticity theory [13]. For the IDB-I_1SF junction line, the initial configurations are based on Volterra models. In both cases the supecells are relaxed to the minimum energy by the use of an interatomic potential.

In order to achieve a satisfactory description of the microstructure and the energetics of junctions between extended defects, a large number of atoms must be taken into account. Although the energies of many of the isolated planar defects observed in epitaxial GaN layers have been determined using *ab initio* calculations, the total energy of large scale atomic configurations involving different planar defects cannot be calculated, for supercells exceed 15,000 atoms. For this purpose, an empirical potential of the Stillinger-Weber type [14], can be employed; this potential has previously been successfully applied for the study of line and extended defects in GaN [15] [16] [17] [18] [19] [20]. The use of an empirical potential in order to describe the structures and energetics of dislocations is certainly less accurate in comparison with a tight-binding approach or *ab initio* calculations, since it does not consider explicitly the electronic effects. Tight-binding or *ab initio* calculations employ mainly two approaches in order to model dislocations. In the first approach a dislocation dipole or multipole is placed in a supercell and this leads to a considerable interaction between dislocations. In the second approach, where an isolated dislocation is considered in a supercell-cluster with periodic boundary conditions along the dislocation line and hydrogen-terminated surfaces parallel to the line direction, the long range elastic effects are not treated rigorously [6] [21] [22]. On the other hand however, in dislocation modeling, medium and long range strain effects play an important role and the empirical potential offers better embedding of the core into the surrounding bulk material. The advantages of the empirical potential calculations are the competency to treat thousands of

atoms and the efficient way to take into account fixed boundary conditions in surfaces parallel to the line direction of the dislocation far from the core area. The strain induced by the dislocation in this case is more accurately estimated. Since the stress of the supercell geometry influences the core structure and the core energy [23], it provides a better embedding of the core. Moreover, such calculations have been proven [24] suitable for treating relatively complicated supercells comprising multiple planar defects.

The material of this highlight has been presented in detail in three regular articles of Physical Review B. The topological analysis of the IDB-SF interactions and the characterization of experimental observations using circuit mapping technique and electron microscopy image simulations has been analysed in ref [25]. The atomic structures and energies of $1/6 < 20\bar{2}3 >$ partial dislocations delineating the I_1 intrinsic basal stacking fault in wurtzite GaN are modelled using an empirical interatomic potential in combination with anisotropic elasticity calculations in ref [26]. Finally the predicted IDB-SF interactions [25] have been analyzed at atomic scale using large scale empirical potential calculations in ref [27].

Our study is divided in two parts. In the first part the $1/6 < 20\bar{2}3 >$ partial dislocations are analysed. In section 2.1 the computational method is given. In section 2.2 the dislocation parameters are calculated using elasticity theory and empirical potential calculations. In the second part and in section 3.1 the topological methodology is outlined and the admissible junctions between IDBs and basal I_1 SFs are determined. The relaxed atomic configurations and their energies are presented in section 3.2. Finally, in section 4 the main conclusions of our study are presented.

2. I_1 SF Partial Dislocations

2.1 Computational Method

The GaN structure (spacegroup $P6_3mc$) [28] consists of four atoms per unit cell and can be visualized as two interpenetrating hexagonal substructures, one of Ga and one of N atoms related by a spacing u along the c-axis. The position vectors of the atoms comprising the crystal's motif are $\mathbf{u}_A = 1/12$ [$40\bar{4}3$], $\mathbf{u}_B = 1/12$ [$\bar{4}04\bar{3}$] for atoms of the one species, and $\mathbf{u}_a = 1/12$ [$40\bar{4}3$] $+ u$ [0001], $\mathbf{u}_b = 1/12$ [$\bar{4}04\bar{3}$] $+ u$ [0001] for atoms of the other species [29]. For the GaN wurtzite structure, $c/a = 1.626$, $u = 0.375$ and the coordination number is 4 [1].

The stacking sequence for the perfect wurtzite structure along [0001] is $\ldots AaBbAaBbAaBb \ldots$, i.e. each layer parallel to the basal plane is composed of two sublayers of distinct atomic species (aB or bA where capital and small fonts denotes distinct atomic species.) (figure 1(a)).

In the wurtzite structure, two types of intrinsic SFs, designated I_1 and I_2, and one extrinsic, designated E, can be formed [13]. These are low-energy defects since they do not disturb the nearest-neighbor packing. The I_1 intrinsic SF (figure 1(b)) corresponds to one violation of the stacking rule and can be formed by the removal of a B plane followed by shearing by $1/3 < 10\bar{1}0 >$ (figure 2).

In order to describe the I_1 SF configuration with bounding partial dislocations, we start from the perfect crystal [13]. Upon removal or addition of a basal disc of atoms (vacancy or interstitial
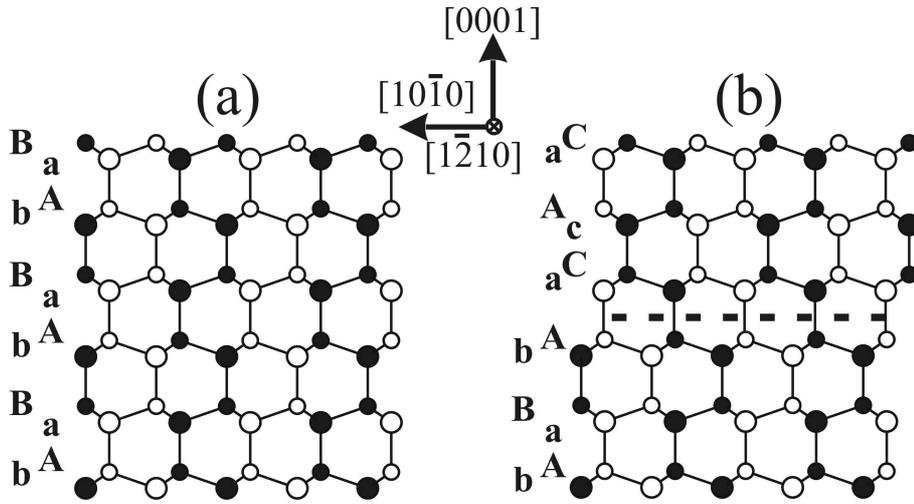
Figure 1: (a) Wurtzite structure and (b) I_1 SF projected along the $< 1\bar{2}10 >$ direction. The broken line indicates the SF plane, large and small circles denote distinct atomic species, unfilled circles are at 0 level, and filled circles are at level $a/2$ along the projection direction.
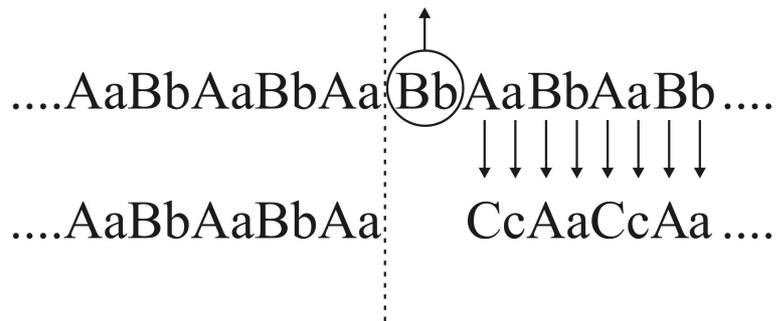
Figure 2: The stacking sequence in the formation of a I_1 SF.

disc) and assuming that only displacements normal to the basal plane are associated with the precipitation, the SF is bounded by a Frank loop with Burgers vectors 1/2[0001] [13]. A loop of Shockley partial dislocation is then nucleated in the faulted region leading to the formation of I_1 SF. In other words, if a shear is associated with vacancy (case a) or interstitial disc precipitation (case b) the I_1 type fault could be formed. The above SFs are bounded by loops comprising edge and mixed segments with Burgers vectors:

$$b_e = 1/2[0001] + 1/3[10\bar{1}0] = 1/6[20\bar{2}3]$$

and

$$b_m = 1/2[0001] + 1/3[1\bar{1}00] = 1/6[2\bar{2}03]$$

respectively (assuming a $[1\bar{2}10]$ segment line direction).

The supercells, for the $1/6 < 20\bar{2}3 >$ edge and mixed partial dislocations, initially contained perfect crystal of wurtzite GaN. By employing displacements expected from anisotropic elacticity theory [13], the unrelaxed structures of the I_1 intrinsic SF and the corresponding partial dislocation were formed to be used as initial atomic positions. The supercells were created in the form of rectangular parallelepiped volumes. Periodic boundary conditions were applied along the dislocation line direction (i.e. $[1\bar{2}10]$), while fixed boundaries were imposed perpendicular to the dislocation line, thus following the so-called "hybrid" model [22]. The fixed boundary conditions were applied using the following methodology (figure 3): perpendicular to the dislocation line the supercell was divided into three concentric domains defining a thin external domain, a thin intermediate domain and the internal area with the dislocation line at the centre. The thickness of the external domain is larger than the maximum range of the potential (3.36 Å for the Ga-Ga interaction [19]), and the atoms are at fixed positions there. The intermediate domain starts at the end of the external one and also extends further than the maximum range of the potential and up to the internal area. In the intermediate domain the atoms are relaxed but are not taken into account in energetic calculations. The energetic calculations are evaluated taking into consideration only the energies of the relaxed atoms in the internal area. (Although test calculations have shown that in most cases the atoms in the intermediate domain are relaxed sufficiently well and their energies could also have been taken into account. It has been found that the deviation of the atomic energies in the intermediate domain, due to their vicinity with fixed atoms, is inversely proportional to the size of the supercell and for the supercells used in the present cases it is very small. Nevertheless the intermediate domain has been excluded from our calculations.)

For the relaxation, the modified [19] [20] Stillinger-Weber potential (MSWp) has been employed. The Stillinger-Weber [14] potential (SWp) attempts to model a semiconductor in a semiclassical way and it is based on a two-body term:

$$\begin{cases} v_2(r_{ij}) = \varepsilon A(B(\frac{r_{ij}}{\sigma})^{-4} - 1)exp[((\frac{r_{ij}}{\sigma}) - \alpha)^{-1}] for \frac{r_{ij}}{\sigma} < \alpha \\ v_2(r_{ij}) = 0 for \frac{r_{ij}}{\sigma} \geq \alpha \end{cases} \qquad (1)$$

and a three body term:
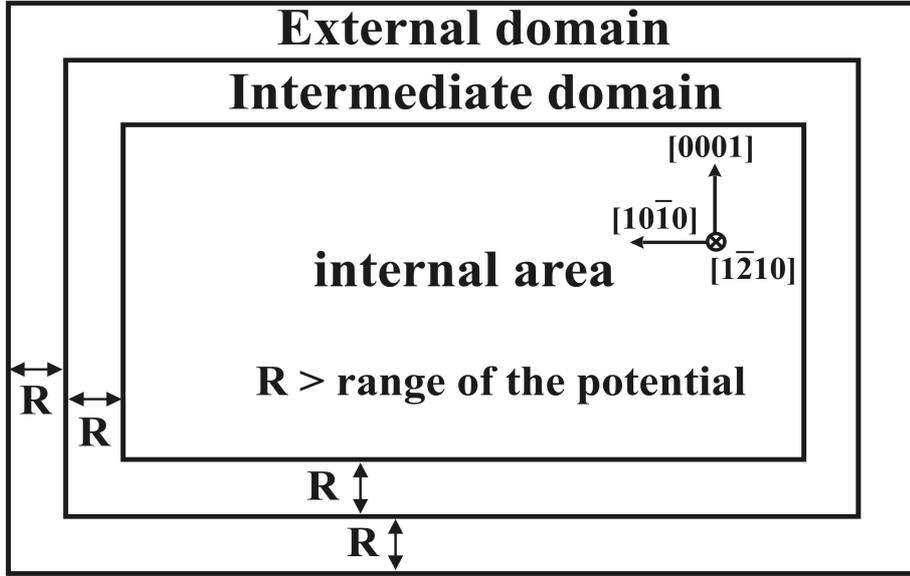
Figure 3: Schematic illustration of the fixed boundary methodology.

$$v_3(r_{ij}, r_{ik}, \theta_{ijk}) = \varepsilon\,\lambda\,\exp[\gamma\,(r_{ij} - \alpha)^{-1} + \gamma\,(r_{ik} - \alpha)^{-1}] \times (\cos\theta_{ijk} + \theta_0)^2 \qquad (2)$$

where ε and σ are the energy and length units; A, B, α are positive, α represents the cut-off distance, and θ_{ijk} is the angle subtended by the ji and the jk bond. The original SWp takes into account 7 parameters (α, γ, σ, ε, A, B, λ). However, its build-in tetrahedral bias of one kind of bonds creates problems in other situations; it is necessary to take into account 21 parameters in order to represent the three kinds of bonds in GaN (*i.e.* Ga-N, and Ga-Ga or N-N "wrong" bonds). In table 1 we present the SWp parameters.

Type of bond	α	γ	σ (a.u.)	ε (eV)	A	B	λ	θ_0
Ga-N	1.8	1.2	3.203	2.17	7.917	0.720	32.50	1/3
Ga-Ga	1.6	1.2	3.968	1.2	7.917	0.720	26.76	1/3
N-N	1.8	1.2	2.457	1.2	7.917	0.720	26.76	1/3

Table 1: Parameters of the modified Stillinger-Weber potential. (α, γ, A, B, λ and θ_0 dimensionless)

The minimum energy configurations were obtained using the quench molecular dynamics method [30]. We assumed bonds between atoms within distances up to 2.4 Å in all atomic configurations which is the minimum range of the MSWp (for the N-N interaction [19]).

Generally, atomistic empirical potential calculations provide the total energy of a relaxed structure. Let E_{TOTAL}^{excess} be the total excess energy of a supercell, defined as the difference between the total energy found by empirical potential calculations and the energy of a supercell of perfect

GaN crystal containing the same number of atoms. Let also $E_{\text{planar defect}}$ be the planar defect energy per unit area, i.e. the total excess energy of a supercell containing the planar defect divided by planar defect area. $E_{\text{planar defect}}$ was evaluated by relaxing a supercell containing a planar defect in the middle; periodic boundary condition were employed along all three directions.

The I_1 SF has been found to have formation energy equal to 1.8 meV/Å^2 which is in satisfactory agreement with the value of 1.1 meV/Å^2 given by *ab initio* [31].

The dislocation energy per unit length, $E_d(R)$, of each dislocation in a cylinder of radius R was calculated as the total excess energy of the cylinder minus the sum of the planar defects energies. Hence

$$E_d(R) = \frac{E_{TOTAL}^{excess}(R) - \sum_{planar\,defects} E_{planar\,defect} \times (planar\,defect_{area}(R))}{L} \tag{3}$$

where L is the length of the supercell along $[1\bar{2}10]$.

Continuum elasticity theory is complementary to atomistic simulations for the modeling of line defects since it allows an evaluation of the long range strain effects whereas atomistic simulations describe core structure and energy. The strain energy of an infinite straight dislocation in a perfect crystal can be calculated analytically using linear elasticity [13]. The total energy of a dislocation is equal to the elastic energy plus the core energy:

$$E_{\text{total}} = E_{\text{elastic}} + E_{\text{core}} \tag{4}$$

The elastic energy per unit length of a dislocation contained in a cylinder of radius R is given by

$$E_{elastic} = A \ln \frac{R}{r_0}, \quad r_0 \leq R \tag{5}$$

where $A = \frac{Kb^2}{4\pi}$ is the prelogarithmic factor, **b** is the Burgers vector, K is an energy factor and r_0 is the core radius.

Let xz be the basal plane where x is $[10\bar{1}0]$, and let the dislocation line $[1\bar{2}10]$ coincide with the z axis. The y axis, in this coordinate system is along the [0001] direction. The elastic energy of a dislocation in the basal plane can be decomposed into screw and edge parts according to anisotropic elasticity as follows [13]

$$E_{elastic} = \frac{1}{4\pi}(K_s b_s^2 + K_{e_x} b_{e_x}^2 + K_{e_y} b_{e_y}^2)ln\frac{R}{r_0} \tag{6}$$

where K_s is the energy factor of b_s, the screw component of the Burgers vector of the dislocation, and K_{e_x}, K_{e_y} are the energy factors of the edge components, b_{e_x} and b_{e_y} respectively.

The energy factors are equal to [13]

$$K_s = (C_{44}C_{66})^{1/2}, \tag{7}$$

$$K_{e_x} = [(C_{11}C_{33})^{1/2} + C_{13}] * \{ \frac{C_{44}[(C_{11}C_{33})^{1/2} - C_{13}]}{C_{33}[(C_{11}C_{33})^{1/2} + C_{13} + 2C_{44}]} \}^{1/2}, \quad (8)$$

And

$$K_{e_y} = [(C_{11}C_{33})^{1/2} + C_{13}] * \{ \frac{C_{44}[(C_{11}C_{33})^{1/2} - C_{13}]}{C_{11}[(C_{11}C_{33})^{1/2} + C_{13} + 2C_{44}]} \}^{1/2} \quad (9)$$

where C_{11}, C_{13}, C_{33}, C_{44} and C_{66} are the elastic constants.

As has been shown previously, two types of admissible partial dislocations may bound the I_1 SF. An edge dislocation with Burgers vector equal to $b_e = 1/6[20\bar{2}3]$ and a mixed-type dislocation with Burgers vector $b_m = 1/6[2\bar{2}03]$. In both cases the dislocation line is taken to be $[1\bar{2}10]$. Using the elasticity theory, the prelogarithmic factors for the edge and the mixed dislocations were calculated, as well as the ratio between them. The edge dislocation can be decomposed into two normal edge components $b_{e_X} = 1/3[10\bar{1}0]$ and $b_{e_y} = 1/2[0001]$ while the mixed dislocation can be decomposed into a screw $b_s = 1/6[1\bar{2}10]$ and two normal edge components $b_{e_X} = 1/6[10\bar{1}0]$ and $b_{e_y} = 1/2[0001]$. Using elastic constants calculated by the MSWp [32], the prelogarithmic factors are found to be $A_e = 0.79$ $eV/\mathring{A}$ and $A_m = 0.73$ $eV/\mathring{A}$ leading to a ratio equal to $\frac{A_e}{A_m} = 1.08$. If experimental determined elastic constants [33] are used the prelogarithmic factors are $A_e = 0.82$ $eV/\mathring{A}$ and $A_m = 0.76$ $eV/\mathring{A}$, and the ratio between them again equals $\frac{A_e}{A_m} = 1.08$, i.e. due to the satisfactory agreement between the experimental and the calculated elastic constants [32], the obtained prelogarithmic factors are also in consistency.

The elastic energy of a dislocation is related to the radius of the cylinder and it is infinite for an infinite crystal. Although it can be calculated for a finite radius, it cannot be considered a characteristic invariable property like the core energy. Therefore, only the dislocation core energy, i.e. the energy of the minimum region which cannot be described by elasticity theory, can be used in such capacity.

In order to evaluate the core parameters of dislocations, the energy in the region bounded by coaxial cylinders of radii r and R_0 is plotted versus $\ln(r)$, where R_0 is the external cylinder radius (taken as large as possible), and r is the internal cylinder radius ($r_0 \leq r \leq R_0$). The core radius r_0 is taken at the point where the curve stops being linear. Equation 5 can be written as:

$$E_{elastic}(r) = A \ln R_0 - A \ln r \quad r \leq R_0. \quad (10)$$

The corresponding prelogarithmic factor is evaluated by fitting equation (10) to the calculated values. The core energy is evaluated by averaging the calculated energy values following equation (3) minus the elastic part:

$$E_d(r) - E_{elastic} = E_d(r) - A \ln r + A \ln r_0. \quad r \geq r_0 \quad (11)$$

2.2 Results

In figure 4 the fully relaxed core structures of all the admissible atomic configurations are presented. Since, in [0001] orientation, the wurtzite structure presents two polarities (N or Ga

polarity), each atomic configuration is relaxed in both cases. In all atomic configurations we have assumed bonds between atoms within distances up to 2.4 Å which is the range of the MSWp for the N-N interaction (although the range for Ga-N and Ga-Ga interactions is larger than 3 Å) [19].

Following the procedure described in the previous section, figures 5 and 6 illustrate the energies $E_{elastic}(r)$ and $E_{core}(r) = E_d(r) - E_{elastic}$ versus $\ln(r)$ plots for partial dislocations delineating a I_1 SF formed by a collapsed vacancy disc or a precipitated interstitial loop respectively. In all cases, it can be observed that the curve becomes linear and the energy assumes the expression given by elasticity theory (eq. 10). In table 2 the calculated core radii, energies and prelogarithmic factors of the analyzed partial dislocations in both polarities of GaN are given. Also the prelogarihmic factors are presented as they have been evaluated by the use of elastic constants calculated with the MSWp ($A_{elastic}^{MSWp}$) and by the experimental elastic constants ($A_{elastic}^{\exp}$).

In the a-edge diagram of figure 5 we notice that the 5/7 core is energetically favorable for both polarities and it exhibits the smallest core radius. In the b-edge case, it is found that, as in a-edge case, the 5/7 core configuration has the lowest energy. These two core configurations are the lowest energy models between all the admissible dislocations and they are the only configurations in which all the atoms are tetrahedrally coordinated. The 8-atom rings (a-edge-b, a-edge-c and b-edge-b) and the 12-atom ring (b-edge-c) configurations include at least one atom with dangling bond and consequently require higher energies.

In the a-mixed diagram of figure 6 it is seen that the a-mixed-b configuration which exhibits a 5/7-atom ring has the smallest core and is energetically favorable. In the b-mixed diagram, it can be seen that the 12-atom ring of the b-mixed-a configuration is energetically favourable and presents the smallest core in comparison with the interstitial type b-mixed-b and c configurations.

Regarding the prelogarithmic factors, the calculated values given in table 2 are in agreement with the elasticity theory calculations. Discrepancies occur between the values for vacancy type b-edge-c configuration, and for, interstitial type, b-mixed-c configurations and the elastic theory calculated values. This divergence is related to the fitting process, in particular in determining the exact value where the curves become linear.

Partial disloca-tion	Core con-figu-ration	r_0 (Å)		E_{core} (eV/Å)		A (eV/Å)		$A_{elastic}^{MSWp}$ (eV/Å)	$A_{elastic}^{\exp}$ (eV/Å)
a-edge-a	5/7	2.0	(2.0)	0.50±0.02	(0.45±0.01)	0.79	(0.76)	0.79	0.82
a-edge-b	8	3.1	(3.1)	1.28±0.02	(1.34±0.02)	0.79	(0.79)	0.79	0.82
a-edge-c	8	3.1	(3.1)	1.34±0.02	(1.39±0.02)	0.78	(0.78)	0.79	0.82
b-edge-a	5/7	2.5	(2.5)	0.72±0.02	(0.76±0.02)	0.78	(0.76)	0.79	0.82
b-edge-b	8	2.5	(3.1)	1.34±0.02	(1.43±0.03)	0.75	(0.78)	0.79	0.82
b-edge-c	12	2.5	(2.5)	1.48±0.01	(1.39±0.01)	0.73	(0.73)	0.79	0.82
a-mixed-a	8	3.1	(3.1)	1.17±0.02	(1.17±0.02)	0.74	(0.74)	0.73	0.76
a-mixed-b	5/7	2.0	(2.0)	0.81±0.02	(0.96±0.02)	0.73	(0.72)	0.73	0.76

a-mixed-c	5/7	2.5	(3.1)	1.30±0.02	(1.48±0.02)	0.73	(0.75)	0.73	0.76
b-mixed-a	12	2.0	(2.0)	0.99±0.02	(1.05±0.02)	0.73	(0.72)	0.73	0.76
b-mixed-b	10	3.1	(3.1)	1.60±0.02	(1.83±0.03)	0.78	(0.83)	0.73	0.76
b-mixed-c	8	3.1	(3.1)	1.77±0.03	(1.66±0.04)	0.81	(0.87)	0.73	0.76

Table 2: The calculated core radii, energies and prelogarithmic factors of the $1/6 < 20\bar{2}3 >$ partial dislocations of GaN in N-polarity. The values for Ga-polarity are given in parentheses. The prelogarihmic factors obtained from anisotropic elasticity by the use of MSWp-calculated elastic constants ($A_{elastic}^{MSWp}$) and by the use of experimental elastic constants ($A_{elastic}^{\exp}$) are given.

In closing the discussion on $1/6 < 20\bar{2}3 >$ partial dislocations we remark that the obtained cores are structurally similar to those found favorable for perfect basal dislocations in GaN by *ab initio* calculations, [22] [34] as discussed in ref [26].

3. IDB-I$_1$ SF Junctions

3.1 Topological Analysis and Computational Method

A rigorous framework for the *a priori* characterisation of defects [29] [35] [36] has been applied in order to determine the defect character of IDB–SF junction lines [25]. This analysis is based on Volterra's description of line defects in elastic continua [37], as extended for bicrystals. For this purpose, the abutting crystal components, designated λ and μ, are initially considered to be joined along their interface with no long-range stresses present (figure 7(a)). A Volterra cut is then introduced along a part of their interface, and the exposed surfaces are modified by the addition/removal of material and/or the application of tractions as shown in figure 7(b). After re-joining the exposed surfaces, a line defect results between the initial interface and the new one. In agreement with the right-handed/finish-start (RH/FS) convention, this defect is described by the rigid-body operation required in order to bring the new μ surface onto the new λ one [29] [35] [36]. Let the new surfaces be obtained from the initial ones by the rigid-body operations $\mathcal{V}(\lambda)_j$ and $\mathcal{V}(\mu)_i$, where $\mathcal{V}(\lambda)_j = (\mathbf{V}(\lambda)_j, \mathbf{v}(\lambda)_j)$ in Seitz notation [38] (with $\mathbf{V}(\lambda)_j$ being the orthogonal part and $\mathbf{v}(\lambda)_j$ the translation part of the operation), and similarly for $\mathcal{V}(\mu)_\rangle$.

Then the line defect is described by the operation [29] [35] [36]

$$\mathcal{Z}_{ij} = \mathcal{V}(\lambda)_j \, \mathcal{P} \, \mathcal{V}(\mu)_i^{-1} \, \mathcal{P}^{-1}, \tag{12}$$

where $\mathcal{P} = (\mathbf{P}, \mathbf{p})$ is the transformation relating the μ coordinate frame to the λ one ($\mathbf{P}$ is the matrix which transforms λ vectors into corresponding μ ones, expressed in the λ frame, and $\mathbf{p}$, is the relative displacement, expressed in the λ frame, of the μ origin away from the λ origin). In the case of dislocations, Eq. (12) yields $\mathcal{Z}_{ij} = (\mathbf{I}, \mathbf{z}_{ij})$, where $\mathbf{I}$ is the identity rotation, and $\mathbf{b}_{ij} = \mathbf{z}_{ij}$ (other admissible types of defects are discussed by Pond [35]). Interfacial dislocations
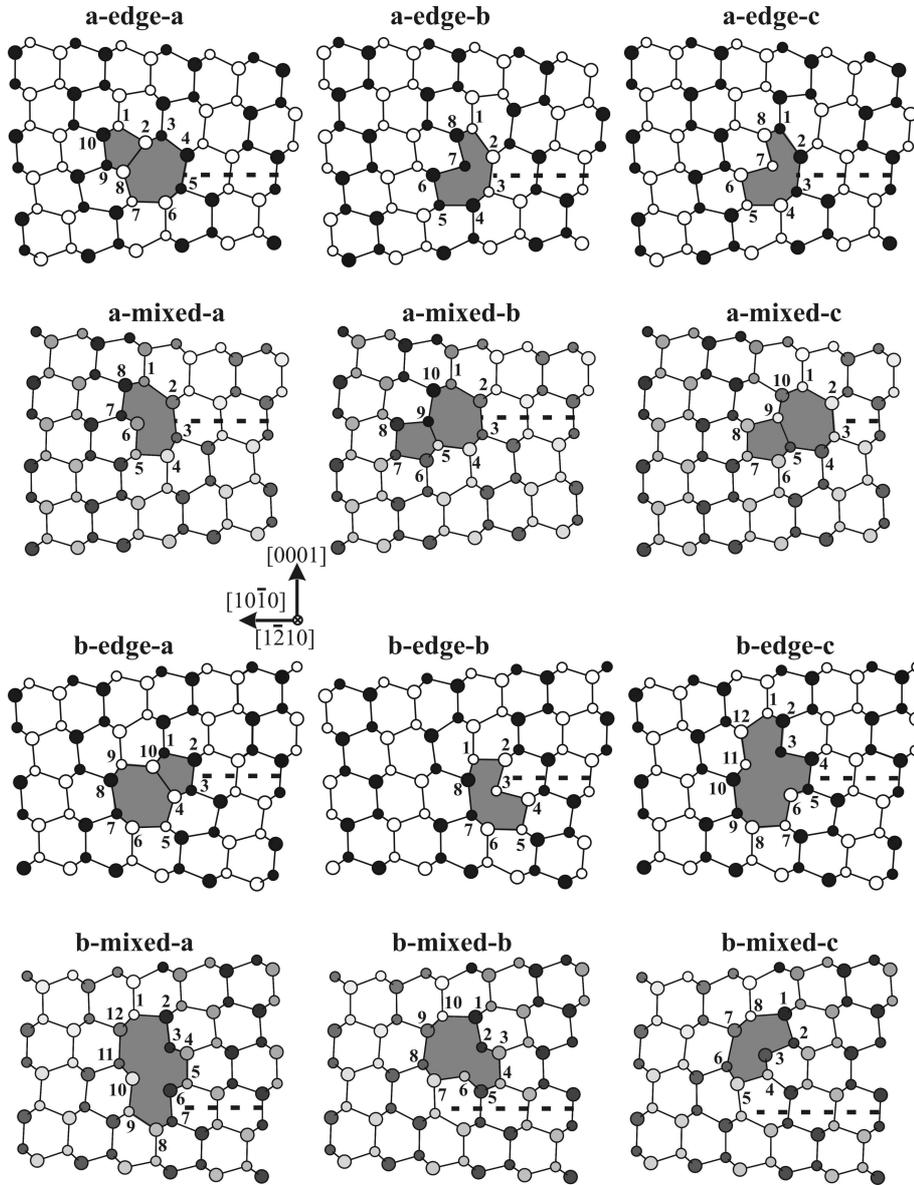
Figure 4: The relaxed atomic core configurations in N-polarity GaN projected along the [1$\bar{2}$10] direction. Symbols are as in figure 1. Shading of atoms indicates distinct levels along the projection direction. For the edge dislocations there are two such levels i.e. at 0 and $a/2$, whereas for mixed type partials shading denotes multiple different levels. The shaded atomic rings depict the cores of the dislocations. Reprinted figure with permission from [26]. Copyright (2004) by the American Physical Society.
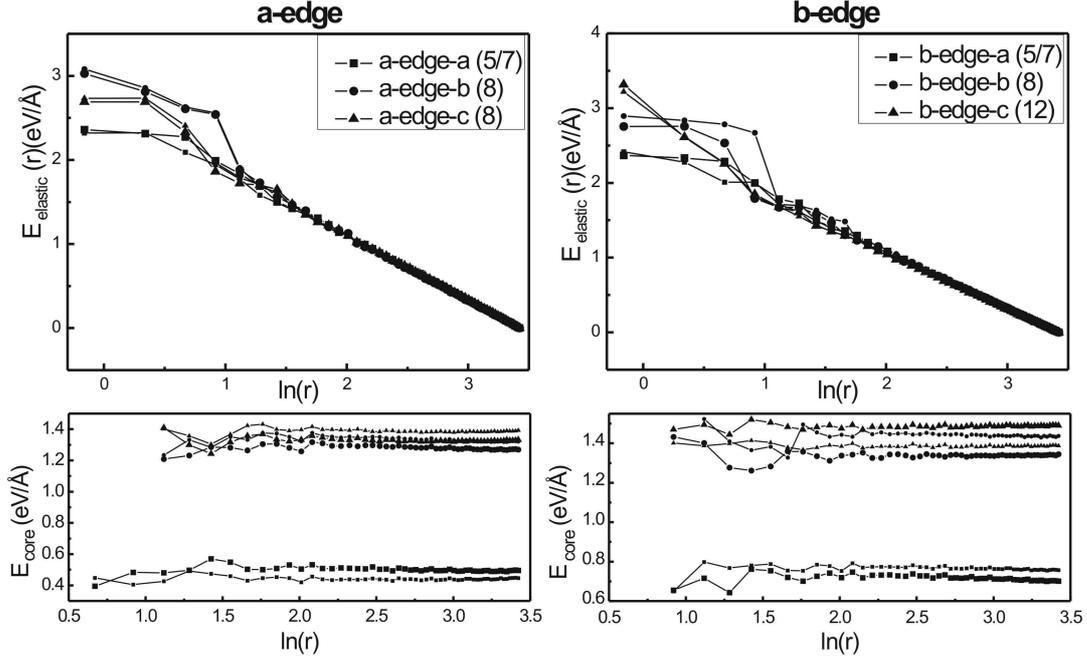
Figure 5: Elastic energy per unit length $E_{elastic}(r)$ stored in the region bounded by coaxial cylinders of radii r and R_0, and the core energy $E_{core}(r) = E_d(r) - E_{elastic}$ as a function of $\ln(r)$ for the a-edge and b-edge configurations. (Large symbols denote N-polarity whereas small symbols denote Ga-polarity) The core radius r_0 is given by the radius below which linearity breaks down. Reprinted figure with permission from [26]. Copyright (2004) by the American Physical Society.
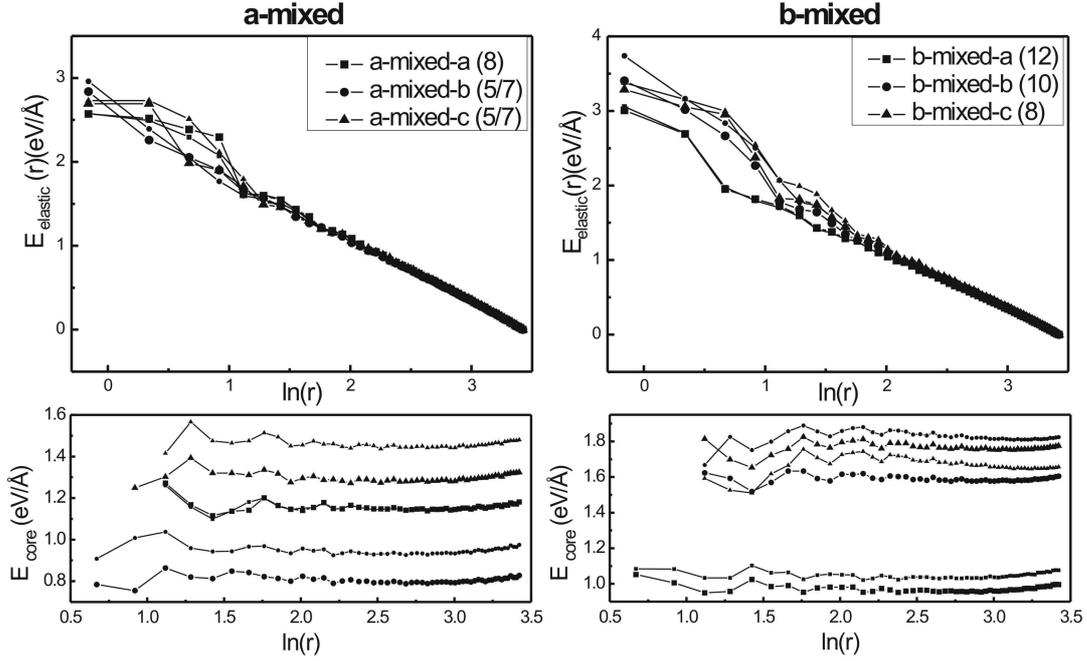
Figure 6: Elastic energy per unit length $\mathrm{E}_{elastic}(r)$ stored in the region bounded by coaxial cylinders of radii r and R_0 and the core energy $\mathrm{E}_{core}(r) = \mathrm{E}_d(r) - \mathrm{E}_{elastic}$ as a function of $\ln(r)$ for the a-mixed and b-mixed configurations. Symbols are as in figure 5. Reprinted figure with permission from [26]. Copyright (2004) by the American Physical Society.
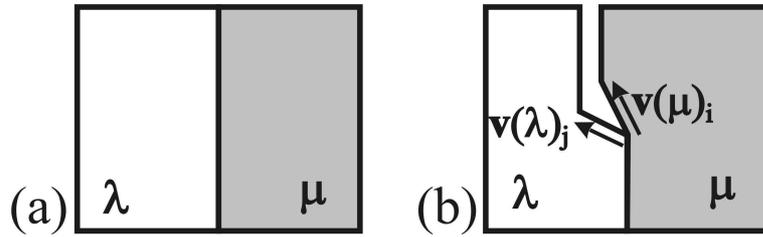
Figure 7: (a) Bicontinuum. (b) Schematic illustration of the introduction of an interfacial dislocation by the Volterra process. Reprinted figure with permission from [25]. Copyright (2001) by the American Physical Society.

can also have associated step character, and this is taken into account by the Volterra approach (figure 7(b)).

In our particular case, we consider the interface to be the $\{10\bar{1}0\}$ IDB and hence $\mathbf{P} = \bar{1}$, the inversion operation, while $\mathbf{p}$ is the relative displacement of the inverse polarity domains. The electronically inert character of one type of inversion domain boundaries (IDBs) has been attributed to a particular relative displacement of the abutting domains leading to the elimination of "wrong" bonds along the IDB plane. Such IDBs have been designated to belong to the IDB* structural model [39] and their observation in GaN specimens has been reported by a number of authors [40] [41] [42]. A second type of IDB, namely the Holt IDB [43], comprises wrong bonds and has been shown to be electrically active [39]. Consequently, it requires a higher formation energy than IDB*s [39]. In figure 8 the atomic structures of the $\{10\bar{1}0\}$ IDB*, and Holt IDB in the GaN wurtzite structure are illustrated. In the $\{10\bar{1}0\}$ Holt-type IDB, $\mathbf{p} = 3/8[0001])$ while, for the IDB*, $\mathbf{p} = -1/8[0001]$. The relative displacement vectors $\mathbf{p}$ are defined taking as reference the Austerman – Gehman IDB model [25] [36] [44].
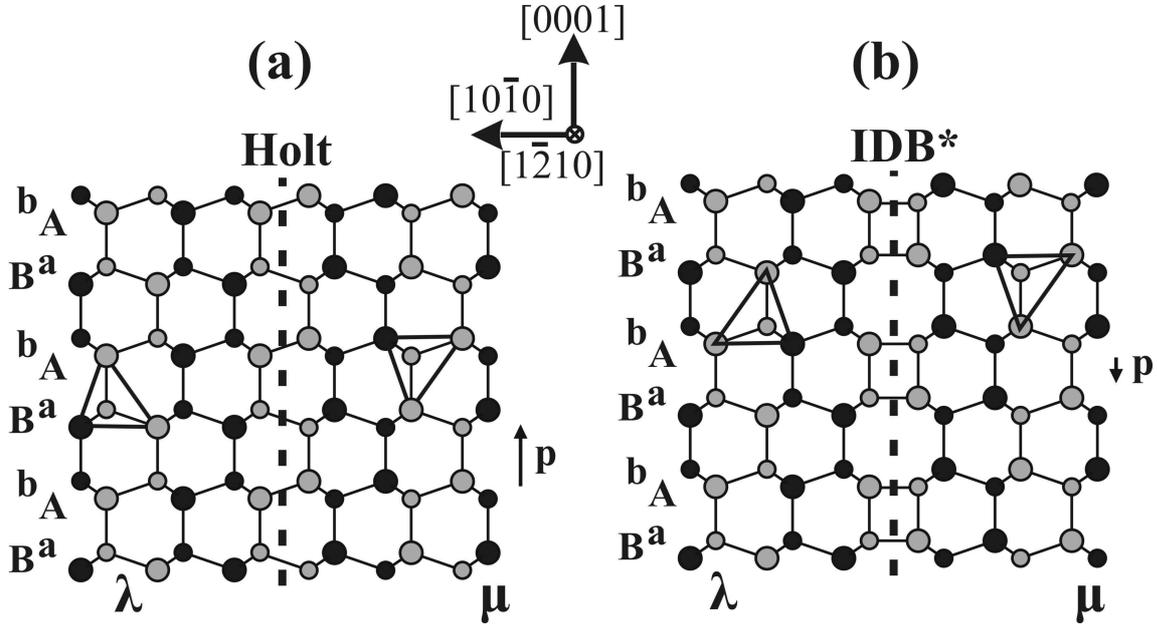
Figure 8: Schematic illustrations of $\{10\bar{1}0\}$ IDBs in the wurtzite GaN structure. (a) Holt-type IDB (p = 3/8[0001]), (b) IDB* (p = −1/8[0001]). ($< 1\bar{2}10 >$ projection, large and small circles denote distinct atomic species, shading indicates levels 0 and $a/2$ along the projection direction, and tetrahedra indicate polarity reversal). The vectors denote displacement of domain μ with respect to domain λ. The stacking sequence along [0001] is also given.

Using the Volterra-like approach, the defect character of IDB junctions with I_1 (0001) SFs can be determined by considering SF-introducing $\mathcal{V}_i$ operations. Two such operations can be distinguished, $i.e.$ either $\mathcal{V}_1 = (\mathbf{I}, \mathbf{v}_1)$ where $\mathbf{v}_1 = \pm 1/3 < 10\bar{1}0 > + 1/2$ [0001], or $\mathcal{V}_2 = (\mathbf{I}, \mathbf{v}_2)$ where $\mathbf{v}_2 = \pm 1/6 < \bar{1}010 > + 1/2$ [0001] $\pm 1/6 < \bar{1}2\bar{1}0 >$. The signs of the $< 10\bar{1}0 >$ components of $\mathbf{v}_1$ and $\mathbf{v}_2$ are reversed when changing the sense of the SF-associated stacking, $i.e. \ldots ABABCBCB\ldots$ or $\ldots ABABACAC\ldots$. The corresponding step heights on the $\{10\bar{1}0\}$

plane are $h_1 = \pm (3)^{1/2} a/3$ and $h_2 = \pm (3)^{1/2} a/6$ respectively.

By employing the aforementioned operations, Volterra-like diagrams of all the admissible junctions of an IDB* with a I_1 SF are illustrated in figures 9(a) to (h), where it can be seen that they lead to transformation of IDB character from IDB* to Holt; the $1/2[0001]$ component of the SF-introducing operation accommodates the IDB structural transformation. In figures 9(a)-(h) we chose to apply the SF-introducing operation to domain μ while, for domain λ, we may employ either the identity operation $(\mathbf{I}, \mathbf{0})$ or a lattice translation $(\mathbf{I}, \mathbf{t}(\lambda))$, where $\mathbf{t}(\lambda) = 1/3< 2\bar{1}\bar{1}0 >$. These operations yield the smallest-in-magnitude Burgers vectors for the particular interactions. The Burgers vectors obtained from Equation (12), as well as the average step heights h_{av} on the IDB plane are also given in figure 9.

In addition to applying the SF-introducing operations only to domain μ, we may apply such operations to both the λ and μ domains (figure 9(i) to (l)). These cases correspond to the SF crossing the IDB, and it can be seen that the IDB type remains invariant. In figures 9(i) and (j), the SF crosses via a dislocation-free step whereas, if the SF structural units are mirror related with respect to the IDB plane, a partial dislocation is required (figures 9(k) and (l)).

For the IDB-SF interactions, the supercells corresponding to each Volterra model have been constructed based on figure 9. The energies of the IDBs that appear in the studied interactions, as calculated by the MSWp [19], are E_{HOLT}=166.3 meV/Å^2 and E_{IDB*}=61.4 meV/Å^2.

In the case of IDB-I_1 SF interaction models, due to the existence of three types of planar defects, there is no linear part in the energy versus $\ln(r)$ plots. Consequently there is no way to evaluate the core parameters but only the prelogarithmic factors by calculating the slope of the fitted line to the curve. The calculated values of the prelogarithmic factors ($A_e = 0.261$ $eV/Å$ for the a-model and $A_m = 0.203$ $eV/Å$ for the f-model) are in satisfactory agreement with the values calculated by elastic theory, ($A_e = 0.258$ $eV/Å$ for edge type and $A_m = 0.245$ $eV/Å$ for mixed type using elastic constants calculated by the MSWp [32],) confirming the coherency of the method.

Taking into account the size of our supercells the interaction energy of each interaction model is equal to the core energy plus an elastic contribution. Consequently the interaction energy represents the core energy of each model and due to the fact that all the supercells have the same size, we are able to compare the calculated values between the models with the same Burgers vector.

3.2 Results

Among the twelve models of figure 9, five comprise edge type partial dislocations (**a**, **d**, **e**, **h**, **l**), five involve mixed type dislocations (**b**, **c**, **f**, **g**, **k**), and two models (**i** and **j**) are dislocation-free interactions. Regarding the two dislocation-free interactions, each case can appear in two possible arrangements of the SF structural units before and after the IDB, thus leading to four initial unrelaxed models (**ia**, **ib**, **ja**, **jb**) [25]. Consequently the total number of Volterra models is equal to fourteen. Additionally by taking into account the polarity of the abutting domains, two atomic configurations, one per each polarity, correspond to each of the fourteen models. Hence a total of twenty eight stable atomic configurations of IDB-SF junctions have been calculated.

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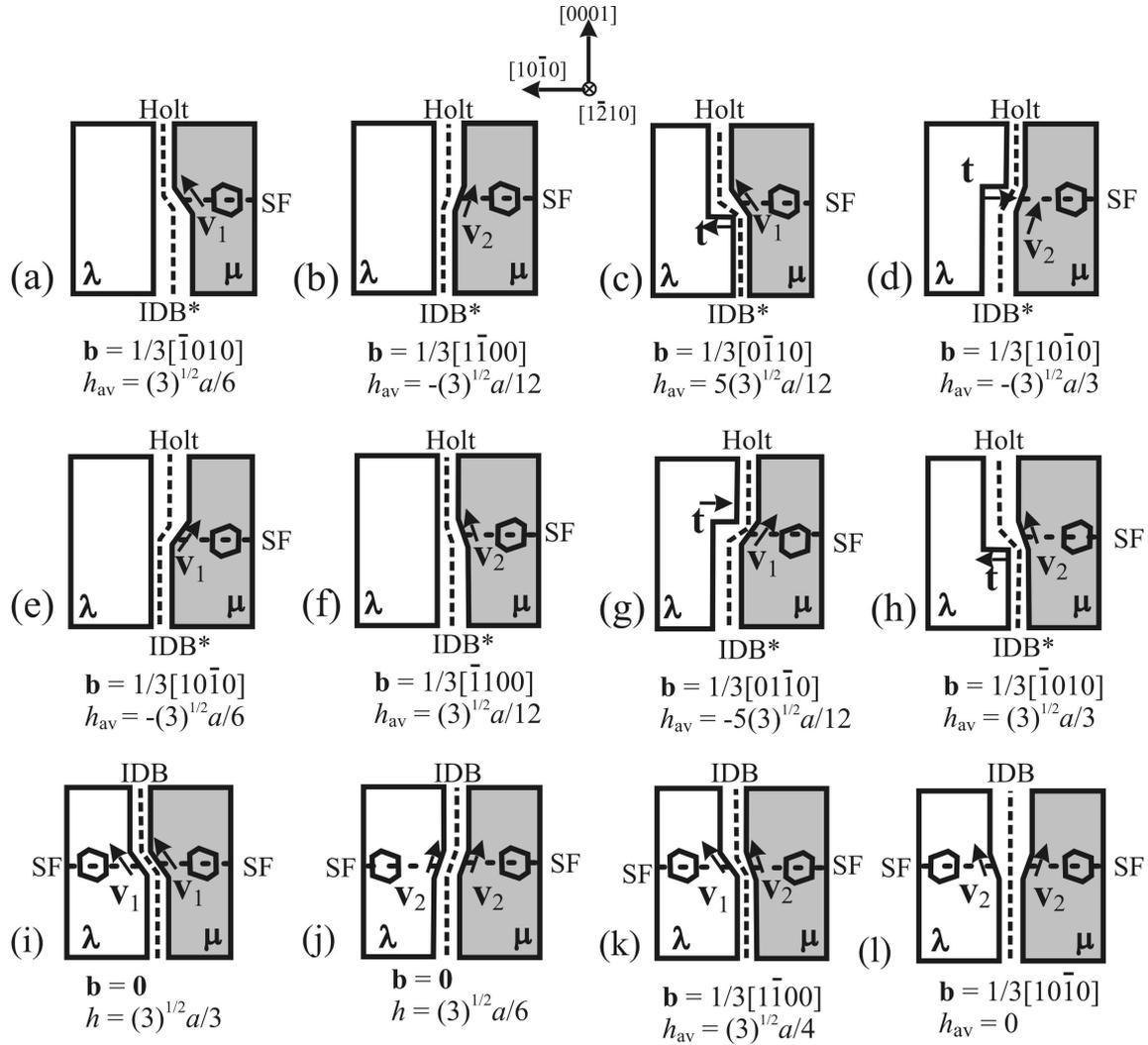
Figure 9: Volterra diagrams of the IDB* - I$_1$ SF junctions. Junctions (a) to (h) lead to a Holt IDB, while configurations (i) to (l) illustrate IDB - I$_1$ SF crossings. The IDBs and SFs have been indicated by broken lines. On each SF, a structural unit has been drawn to indicate its sense. The given configurations correspond to minimum Burgers vectors and minimum average step heights (h$_{av}$). Reprinted figure with permission from [25]. Copyright (2001) by the American Physical Society.

The models **i**, **j**, **k**, and **l**, where the SF crosses the IDB without transforming its character, may be constructed either with IDB* or Holt type IDB. In the present study we examine only crossings involving IDB*s since they are energetically more favourable than Holt IDBs [39].

a) Edge type partial dislocations

The energy calculations indicate that the **a** model has the lowest energy of the edge type models. The relative energies ΔE_{Jn} for the stable atomic configurations of the **a**, **d**, **e**, **h**, and **l** models, taking as reference the lowest energy, are given in figure 10. The associated junction line defects are edge partial dislocations with Burgers vector $b_e = 1/3\,[10\bar{1}0]$.
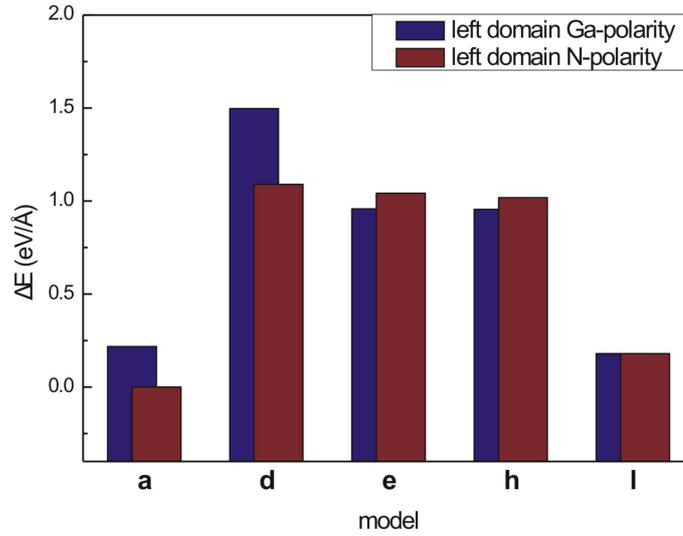
Figure 10: Relative energies calculated by the MSWp, for both polarities of the models a, d, e, h and l. The associated partial dislocations have edge character.

The corresponding relaxed atomic configurations are presented in figure 11.

b) Mixed type partial dislocations

In interactions where the associated junction line defects are partial dislocations with mixed character (i.e. **b**, **c**, **f**, **g**, and **k**) the Burgers vector can be decomposed into a screw $b_S = 1/6\,[1\bar{2}10]$ and an edge component $b_e = 1/6\,[10\bar{1}0]$. The relative energies as calculated by the MSWp, and taking as reference the lowest energy (**k** model), are given in figure 12.

In figure 13 the relaxed atomic configurations of the models **b**, **c**, **f**, **g** and **k** are presented.
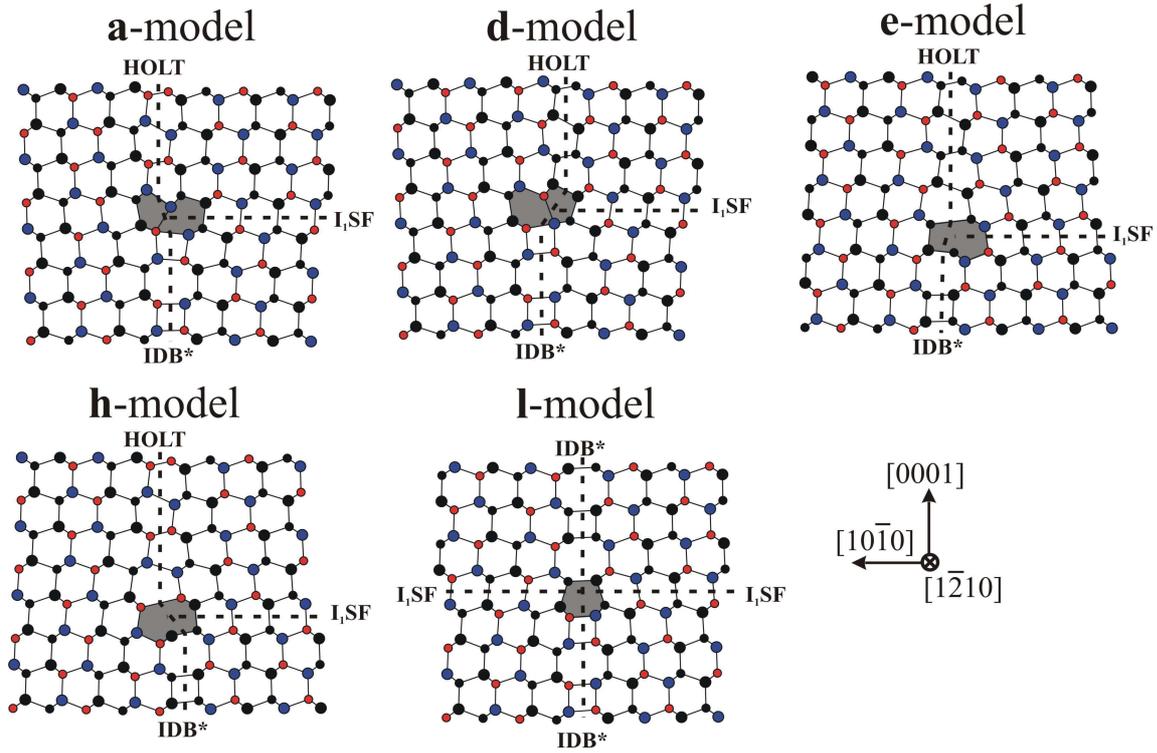
Figure 11: Relaxed atomic configuration of models a, d, e, h and l given in figure 9, which comprise interactions involving partial dislocations with edge character. ($< 1\bar{2}10 >$ projection, broken lines indicate planes of IDBs and SFs, large and small circles denote distinct atomic species, shading of atoms denotes levels 0 and a/2 along the projection direction and the shaded areas represent the central atomic rings of the cores).
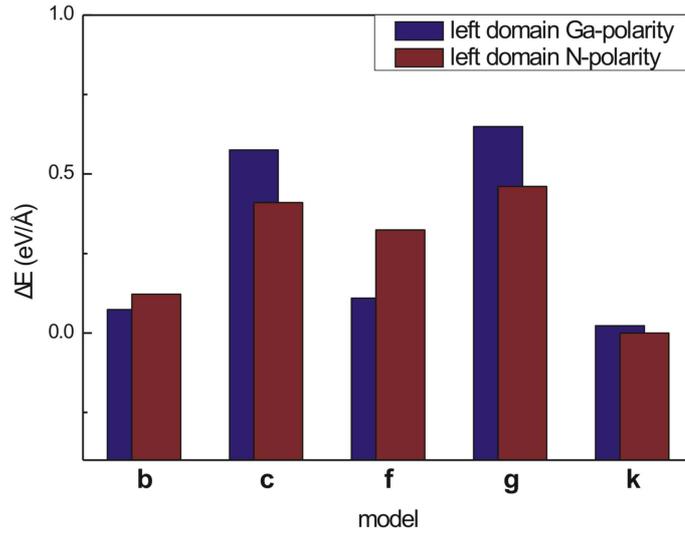
Figure 12: Relative energies of models b, c, f, g, k calculated by the MSWp. The associated junction line defects are mixed type dislocations.
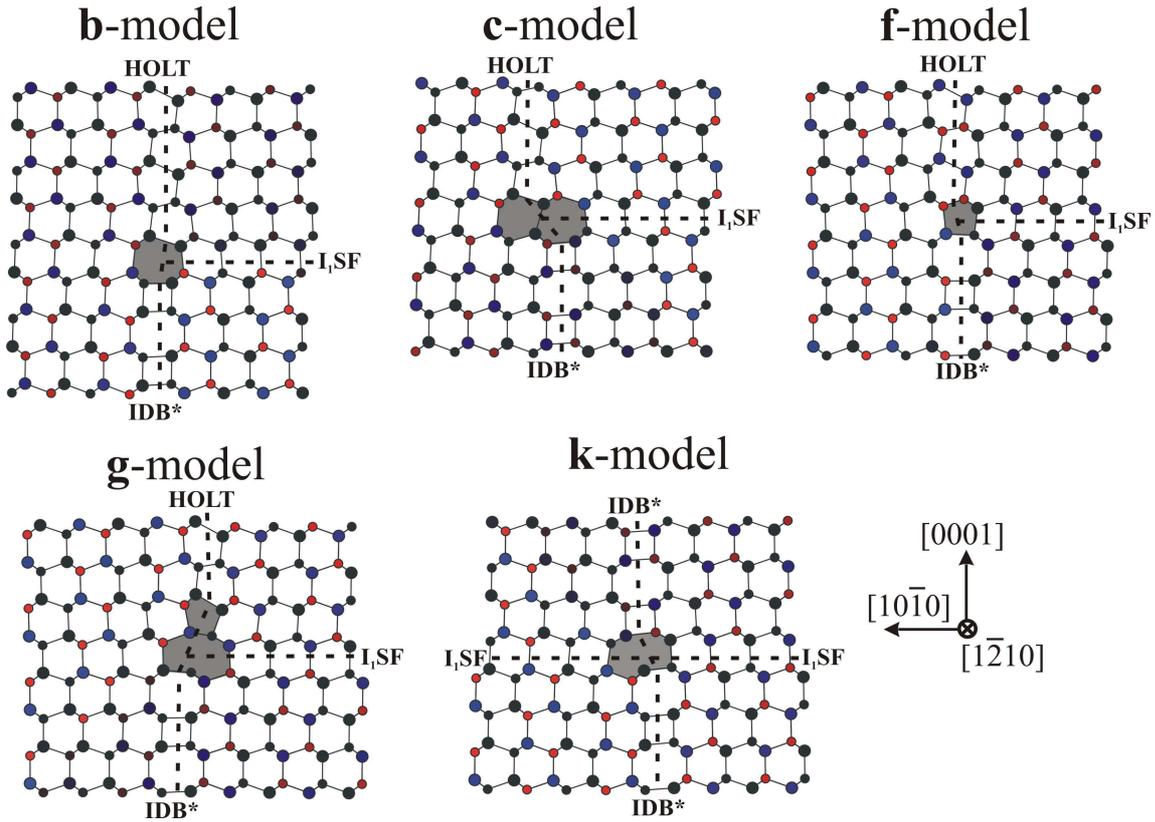
Figure 13: Relaxed atomic configuration of models b, c, f, g and k given in figure 9, which comprise partial dislocations with mixed character. ($< 1\bar{2}10 >$ projection, atoms and symbols are as in figure 11).

c) Dislocation-free interactions.

Two dislocation-free IDB-I$_1$ SF junctions have been depicted in figure 9 (models **i**, **j**). As it has already been pointed out, each case comprises two possible stable arrangements of the SF structural units before and after the IDB, leading to four models (**ia**, **ib**, **ja**, **jb**) [25]. The relative energy of each configuration, taking as reference the lowest energy, was calculated for both polarities of GaN and the corresponding values are presented in the bar-graph of figure 14.
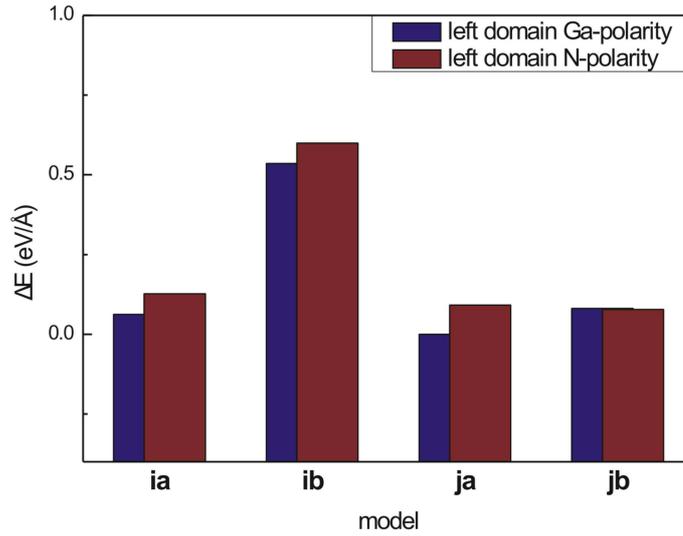
Figure 14: Relative energies of dislocation-free junctions calculated by the MSWp.

In figure 15, the relaxed atomic configurations are presented.

We have presented so far the admissible IDB-SF junctions and a detailed analysis based on the MSWp potential have been presented in ref [27]. It has to be noticed that although the MSWp yields about the maximum accuracy currently possible for the given model sizes, especially for GaN with bulk like coordination of atoms, the energies of the reconstructed cores comprising of Ga-Ga and N-N bond are less accurately represented. However the relaxed models can be used as reference for band structure calculations.

Almost all the relaxed core structures comprise a 5 or 7-atom ring.

Moreover in ref [27], one of the determined core structures has been matched to an IDB-SF junction line observed by high resolution transmission electron microscopy. In particular, this was achieved for the **f**-model which has the second lower energy for the mixed type partial dislocations leading to IDB* transformation to Holt IDB.
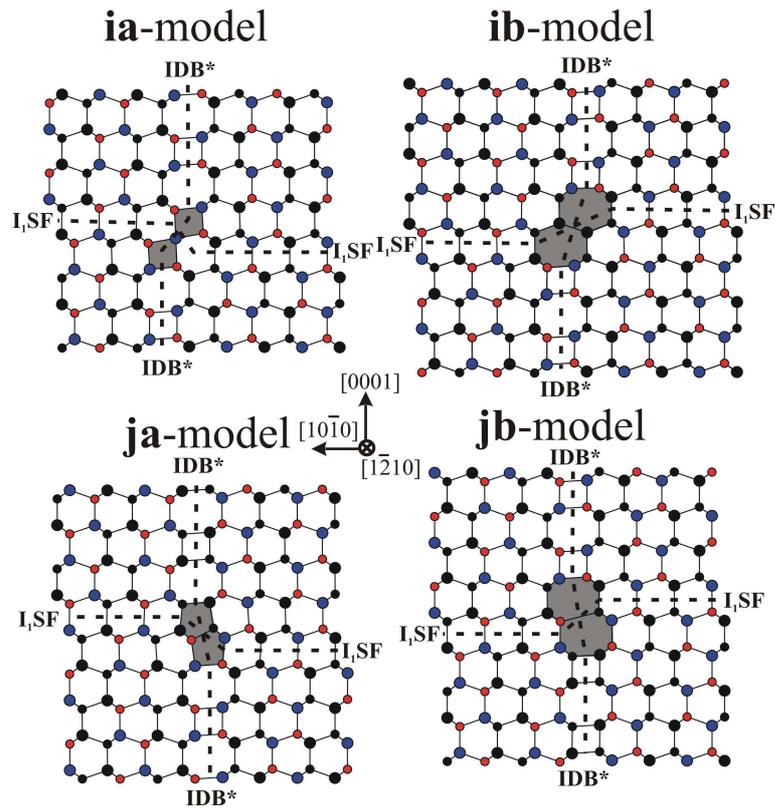
Figure 15: Relaxed atomic configurations of models i and j (figure 9) which comprise dislocation-free interactions. ($< 1\bar{2}10 >$ projection, atoms and symbols are as in figure 11).

4. Conclusions

The atomic structures and dislocations parameters of the $1/6 < 20\bar{2}3 >$ partial dislocations that bound the I_1 SF and the $1/3 < 10\bar{1}0 >$ admissible partial dislocations at the junction lines between I_1 SFs and IDBs have been calculated by means of empirical potential calculations in combination with topological and elastic theory.

Our calculations on $1/6 < 20\bar{2}3 >$ partial dislocations reveal twelve stable configurations in each polarity and their core structures and energies have been presented. Although there are difficulties in determining the exact cylinder radius below which linearity breaks down the core radii have been calculated in the range between 2 and 3.1 Å, and, in all cases, the smallest cores belong to the energetically favourable configurations.

The 5/7 ring core in which the atoms are tetrahedrally coordinated has been found energetically favourable among the edge configurations; such cores have been calculated, in all cases, to have energies less than 0.76 eV/Å. The 8- and 12-atom rings have been found to require energies from 1.28 to 1.48 eV/Å.

Regarding the mixed type partial dislocations, a variety of core configurations (8, 5/7 and 12 atom rings) has been revealed. The 5/7- and 12-atom ring configurations has been found favorable for partial dislocations delineating a I_1 SF formed by a collapsed vacancy disc or a precipitated interstitial loop respectively. However, none of them has been found to consist of only tetrahedrally coordinated atoms. Their core energies are larger than the edge type dislocations and the energetically favourable models were found to require energies from 0.81 to 1.05 eV/Å.

Based on the analysis of ref [26], it is reasonable to postulate that $1/6 < 20\bar{2}3 >$ partial dislocations in wurtzite GaN may introduce band gap states. However, in addition to the core structure, the strain environment in the surrounding crystal plays an important role. Further investigations are required in order to determine their influence on the band structure.

Regarding the IDB-I_1 SF interactions, twenty eight stable configurations of such junctions have been identified, sixteen of them resulting in transformations of IDB* to Holt IDBs. Consequently, the IDB*-I_1 SF interactions appears to be an important mechanism for the introduction of Holt IDBs.

Moreover, the majority of the core structures exhibit either dangling bonds or highly distorted bond angles and lengths [27]. Since gap states may arise from reduced coordination or strained bonds, these dislocations could be electrically active. Furthermore the core stress field could act as a trap for electrically active native defects (e.g. vacancies) or impurities. Consequently almost all the examined junction cores are potentially electrically active defects.

It has also been found that the core energy depends on polarity for dislocations with line direction along $< 1\bar{2}10 >$ [26], [27]. When the polarity of the supercells is inverted, the core ring configuration remains invariant but not the lengths of the bonds and the angles between them. The changes depend on the type of the atoms and the positions of their neighbour atoms.

5. Acknowledgements

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