Scientific report

on the International Workshop on "Multiscale Modeling of Extended Defects and Phase Transformations at Materials Interfaces"

Place :	University of Wrocław, Wrocław, Poland
Date :	September 24-26, 2006
Sponsors :	Psi-k Programme "Towards Atomistic Materials Design"; COST Action P19: "Multiscale modeling of materials"; University of Wrocław
Organizers :	Adam Kiejna, University of Wrocław, Poland; Mojmir Šob, Masaryk University Brno, Czech Republic
Web Page :	`http://www.ifd.uni.wroc.pl/mmds-wroclaw/`

Summary

In order to understand in detail industrially relevant processes such as mechanical properties and fracture, chemical reactions at surfaces, micromagnetism, and polymer processing one has to combine different time and length scales. The aim of the workshop was to bring together distinguished representatives of physics, chemistry, materials science, and metallurgy communities to present and discuss state-of-the-art developments and the perspectives of theory, techniques, and applications, in multiscale modeling of such processes.
The programme of the workshop has included both the activities of the WG6 and WG15 of the Psi-k Network and of the COST Action P19 "Multiscale modeling of materials". During three full days of the workshop (Sunday through Tuesday) there were 19 keynote invited talks (40 min.), presented by internationally well-recognized speakers. These invited lectures were accompanied by 5 contributed talks (20 min.) and by 20 posters, which were presented by young participants of the Workshop. The total attendance of the Workshop was 60 registered participants from 16 countries, including 30 junior scientists (PhD students or post-docs). An important part of the workshop were two panel discussions entitled "Multiscale modelling, where do we stand". The first part was moderated by Prof. Sidney Yip (MIT Cambridge, USA), the second part, concluding the Workshop, by Prof. Matti Alatalo (Lappeenranta University of Technology, Finland), the Chairman of the COST Action P19: Multiscale Modelling of Materials.

Description of the scientific content

A brief summary of the invited talks is as follows:
Sidney Yip described a class of atomic and charge transport problems at the interface of chemical physics and materials science where electronic-level calculations and atomistic calculations required to resolve the basic mechanisms.
Jörg Neugebauer discussed the key role of extended defects and grain boundaries in grain growth and recrystallization and recalled the importance of grain-boundary engioneering.

Igor Abrikosov presented an overview of recent theoretical results in the field of first-principles simulations of phase stabilities of alloys. The first-principles approach is combined with the statistical mechanics within the Ising Hamiltonian with parameters determined ab initio, and the Monte-Carlo method is applied.
François Willaime presented a systematic study of the structure and migration of small defect complexes in Fe from first principles. The results enabled an improvement of empirical interatomic potentials for iron and its alloys by including the first-principles results on defect properties into the database used for the fitting the potentials.
Gabor Csanyi presented recent developments in atomistic hybrid QM/MM simulation methodology, focussing on the problematic areas of matching at the boundary between the classical and quantum-mechanical regions.
Takayuki Kitamura was discussing the strength of interface edge in small (nanoscale) components. He discussed the delamination of cracks at the "interface edges", the junctions, where an interface meets a surface or another interface.
Mikko Alava dealt with statistical physics of material with defects; the main subject of his talk was the strength of brittle materials and the role of disorder.
Adrian Sutton reviewed recent results regarding the structure of twist grain boundaries in silicon. He discussed new, lower energy and ordered configurations of these grain boundaries.
Risto Nieminen reported first-principles calculations of the structure and electronic properties of several different silicon-hafnia interfaces. The simulations show that oxygen always diffuses towards the interface to form a silicon dioxide layer.
Dieter Suess discussed a micromagnetic model allowing for the calculation of process of information writing in the magnetic recording devices. This multiscale method may be applied to design advanced magnetic recording media.
Oksana Chubykalo Fesenko outlined the development of an atomistic model of magnetisation process and applied it to calculations of static and dynamical magnetic properties of nanogranular FePt. She demonstrated finite-size effects in elements used for magnetic recording.
Yuan Ping Feng proposed a new method for chemical tuning of metal effective work function at the interfaces between a high-K oxide and a metal gate. His approach was illustrated at the Ni/HfO2/Si stacks.
Guy Courbebaisse reviewed applications of the lattice Boltzmann method in the field of fluid mechanics. It also enables to use microsopic models to simulate macroscopic behaviour of fluid flows. As an illustration, he presented polymer injection moulding, where some industrial applications may be expected.
Dieter Wolf demonstrated how the materials-physics based insights into the underlying deformatioon and grain-growth mechanisms extracted from molecular dynamics simulations can be incorporated into a mesoscopic simulation model, overcoming the length and time-scale limitations inherent to the molecular dynamics approach. As an example, he discussed diffusion creep in a material containing a large number of grains with arbitrary sizes.
Göran Wahnström presented ab initio results for interfaces in two different systems: sintered WC-Co cemented carbides and ferritic steels. He showed the findings of a quantitative analysis of WC grain shape using the density functional theory and transmission electron microscopy. In steels, he considered VN presipitates which form platelets in ferrite due to a small (2 misfit parallel to the platelet and appreciable misfit (44 the platelet.

Karsten Reuter sketched multiscale modeling attempts for the field of heterogenous catalysis, concentrating particularly on the relevance of treating the surrounding gas phase, as well as the statistical interplay of the manifold of elementary processes at a catalyst surface. He also discussed atomistic thermodynamics.
Vasyl Tokar presented a lattice gas model of coherent strained epitaxy and discussed the size calibration od self-assembled nanoparticles. He was able to explain the discrepancy between the low atomic mobility predicted by a naive application of the ab initio approach and the high mobility presented experimentally.
Matous Mrovec reviewed the theoretical background of bond-order potentials and discussed the latest developments. The applicability of the bond-order potentials was demonstrated by several examples of studies of extended defects, in particular dislocations and grain boundaries which control the mechanic properties in metallic systems.
Vaclav Paidar compared various approaches to the grain boundary classifications and the interpretation of recent experimental results in the context of the complex relationship between microstructure, local chemistry and material properties. Such findings are essential for grain boundary engineering proposed to improve the performance of polycrystalline materials.

Panel discussion: Summary
The first part of the panel discussion was moderated by Sidney Yip. The panelist were François Willaime, Dieter Wolf and Adrian Sutton. **François Willaime** dealt with materials under irradiation. These materials exhibit non-equilibrium steady states and there are complex phenomena to be studied. Ab initio calculations often reconcile simulations with experiments. Computer simulations are increasingly important in the field of materials under irradiation and there are numerous international initiatives: CEA/Saclay & UK (Culham), European Fusion and Fission Project (since 2004), collaboration between the USA and CEA, between the EU and Japan etc. **Dieter Wolf** indicated that computer simulations are rather complementary to experiment. In the multiscale modelling, a great challenge is the time-scale problem. We have defined greater and greater details which we know with the double precision. Everyone giving a simulation talk should state how the results can be used e.g. for higher-level simulations - definitely not the pictures! It should be clearly indicated what can be passed to a higher level. **Adrian Sutton** summarized the main problems in the multiscale modelling:

1. Grand-canonical simulations for interfaces

2. Fracture toughness of polymer-inorganic interfaces and of nanocomposites

3. Beyond Ehrenfest non-adiabatic simulations with excited electrons

4. A continuing need for simple models to gain insights into complex materials and processes, e.g. (a) TB vs. DFT, (b) a possibility for massive simulations of radiation damage and defect processes in ferromagnetic iron

5. Education and training in Materials Modelling. Materials Science and Modelling has been diversified and post-graduate education would be desirable. Recent example: About 5 institutions in London try to share lessons and seminars and provide eduvation and training for students of MSE in UK.

6. Disconnect between fashion and industrial requirements: we need to look outwards and not inside. Materials Modeling seems to be divorced from the needs, seems to be "self-oriented". Challenges in real life are often different from those pursued in materials modelling community.

Part two of the panel discussion was moderated by Matti Alatalo. First, he has given information about the COST Action P19: Multiscale Modelling of Materials (MMM). It is possible to include projects in MMM into this Action. He also announced a Summer School on MMM. It will take place in Lappeenranta, May 23-26, 2007. It should be reasonably cheap and nice to visit, also e.g. in the range of short-term scientific mission within the above-mentioned COST Action P19. **Josef Fidler** informed about the activity of the WG3 (Micromagnetism) of the COST Action P19. At present, about 10 groups are participating. **Guy Courbebaise** outlined the activities of the WG4 on Hybrid Simulation Methods (COST Action P19). In particular, he showed the possibilities of the lattice Botzmann method in the field of fracture in solids. **Matti Alatalo** presented some thoughts of **Mike Finnis**, who could not attend the Workshop. His views concerned hybrid vs. hierarchical modelling and some examples of problems belonging to one or other mode of modelling. **Marc Hou** informed the other participants about an European initiative on radiation damage.

Assesment of the results

The primary goal of the Workshop, namely to provide a forum for the exchange of ideas on state-of-the-art developments, perspectives, and challenges of multiscale modeling at materials interfaces was fulfilled. Let us note that especially young participants of the Workshop benefited a lot from the Workshop. They had a possibility of a direct contact with the leading experts in the field and most of them could present their results. Discussions at posters brought them new ideas for their future work.
The challenges to be faced and the future directions of research in multiscale modelling have been discussed during the panel discussion (for summary see above).

Final programme

Sunday, September 24

9:00 – 10:00 Registration

10:00 – 10:05 Opening

10:05 – 10:45 X. Lin, J. Li, X. Qian, C. Först, Sidney Yip (Cambridge, USA)
Multiscale Materials Modeling of Reactive Transport

10:45 – 11:25 Jörg Neugebauer (Düsseldorf, Germany), L. Lymperakis
Extended defects and grain boundaries in Al-based materials

11:25 – 11:40 Coffee/tea break

11:40 – 12:20 Igor Abrikosov (Linköping, Sweden)
Phase stabilities and phase transformations in alloys from first-principles

12:20 – 13:00 François Willaime (Saclay, France)
Structure and mobility of defect clusters and defect complexes in iron from first principles

13:00 – 15:00 Lunch

15:00 – 15:40 Gabor Csanyi (Cambridge, UK)
Hybrid classical and quantum-mechanical molecular dynamics simulations

15:40 – 16:10 Coffee/tea break

16:10 – 16:50 Takayuki Kitamura (Kyoto, Japan)
Strength of Interface Edge in Small Components

16:50 – 17:30 Mikko Alava (Helsinki, Finland), P. Nukala, S. Zapperi
Statistical physics of materials with defects

17:30 – 19:00 Poster session/ snacks

Monday, September 25

9:15 – 9:55 Adrian P. Sutton (London, UK), S. von Alfthan, K. Kaski
Twist boundaries in silicon: a new look at an old problem

9:55 – 10:35 Risto M. Nieminen (Helsinki, Finland), M. H. Hakala, A. S. Foster
Modeling the silicon-hafnia interface

10:35 – 11:00 Coffee/tea break

11:00 – 11:40 Dieter Suess (Vienna, Austria)
Multiscale modeling of advanced magnetic recording devices

11:40 – 12:20 R. Chantrell, U. Nowak, Oksana Chubykalo-Fesenko (Madrid, Spain)
Modelling of the dynamic properties of structured magnetic materials

12:20 – 13:00 Panel discussion I: *Multiscale modelling, where do we stand?*
Moderator: Sidney Yip (Cambridge, USA)

13:00 – 15:00 Lunch

15:00 – 15:40 Yuan P. Feng (NUS, Singapore), Y.F. Dong, Q. Li, Y.Y. Mi, S.J. Wang, C.K. Ong, A. Huan
First-Principles Study on Interfaces of High-K Oxides with Silicon and Metal Gate

15:40 – 16:20 Guy Courbebaisse (Lyon, France)
The Lattice Boltzmann Method

16:20 – 16:40 Coffee/tea break

16:40 – 17:00 Andreas Pedersen (Reykjavik, Iceland), G. Henkelman, J. Schiøtz, H. Jónsson
Long Time Scale Simulations of Atomic Structure and Dynamics at Defects in Metals

17:00 – 17:20 P. Piekarz, Krzysztof Parliński (Cracow, Poland), A.M. Oleś
The mechanism of Vervey transition in magnetite Fe_3O_4

17:20 – 17:40 Victoria Yardley (Sendai, Japan), H. Fujii, S. Tsurekawa
Modelling magnetic field effects on the crystallisation of amorphous Fe-Si-B alloys

19:00 – Conference dinner

Tuesday, September 26

9:15 – 9:55 Dieter Wolf (Idaho Falls, USA)
Atomistically-informed Mesoscale Simulation of Grain Growth and Grain-boundary Diffusion Creep in Nanocrystalline Materials

9:55 – 10:35 Göran Wahnström (Gothenburg, Sweden)
Ab-initio studies of interface energies

10:35 – 11:00 Coffee/tea break

11:00 – 11:40 Karsten Reuter (Berlin, Germany)
First-Principles Statistical Mechanics Approaches to Heterogeneous Catalysis

11:40 – 12:20 Vasyl I. Tokar (Strasbourg, France), H. Dreyssé
Fracture of coherent nanoislands during submonolayer strained epitaxy

12:20 – 13:00 Matous Mrovec (Freiburg and Karlsruhe, Germany), C. Elsaesser
Bond-order potentials for simulations of phases, interfaces and dislocations in metallic and covalent materials

13:00 – 15:00 Lunch

15:00 – 15:40 Vaclav Paidar (Prague, Czech Republic), P. Lejček
Segregation to grain boundaries of different types

15:40 – 16:00 Antti Puisto (Lappeenranta, Finland)
Cu oxidation: effect of surface modifications

16:00 – 16:20 E.E. Zhurkin, T. Van Hoof, Marc Hou (Brussells, Belgium)
Modelling plasticity and superplasticity of cluster assembled nanoalloys

16:20 – 16:40 Coffee/tea break

16:40 – 18:00 Panel discussion II: *Multiscale modelling, where do we stand?*
Moderator: Matti Alatalo (Lappeenranta, Finland)

Posters

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1. Juan Beltran (Madrid, Spain), M.C. Muñoz
   Adhesion at transition metal-ZrO_2 interfaces

2. Miroslav Čák (Brno, Czech Republic), M. Šob, J. Hafner
   First-principles study of the $\Sigma5(310)$ grain boundary in iron

3. Christopher W.M. Castleton (Uppsala, Sweden), A. Höglund, S. Mirbt, K. Hermansson
   Scaling the supercell errors in charged defect calculations: Correlations, band gaps and the LDA dielectric constant

4. Miroslav Cerny (Brno, Czech Republic), J. Pokluda
   First Principles Study of Vanadium Based Composites Reinforced by Tungsten Nano-fibres

5. Maria G. Ganchenkova (Helsinki, Finland), V.A. Borodin, S. Nicolaysen, and R. M. Nieminen
   Planar vacancy cluster formation in a non-hydrostatically loaded Si and SiGe crystals

6. Jerzy Gawd (Cracow, Poland), M. Pietrzyk
   Multiscale CAFE model of hot working process accounting for dynamic recrystallization

7. Jana Houserová (Brno, Czech Republic), M. Šob
   Ab initio study of thermodynamics and structure of Ta-X (X=Cr, Fe, W) C14 Laves phases

8. Karen Johnston (Espoo, Finland), R. M. Nieminen
Understanding Polymer Adhesion: First-principles Calculations of the Adsorption of Organic Molecules onto Si Surfaces

9. Jan Kuriplach (Prague, Czech Republic), O. Melikhova, M. Šob
Magnetic moment and segregation at selected grain boundaries in nickel

10. Dominik Legut (Brno, Czech Republic), M. Šob
Magnetism along ideal tensile tests of Ni_3Al and Fe_3Al

11. Tomasz Ossowski (Wrocław, Poland), A. Kiejna
Surface and $\Sigma 5(210)$ *grain boundary properties of chromium*

12. Tomasz Pabisiak (Wrocław, Poland), A. Kiejna
One-dimensional Au on rutile $TiO_2(110)$

13. Grzegorz Pawlik (Wrocław, Poland), A. C. Mitus
Monte Carlo study of diffraction gratings in azopolymers

14. P. Scharoch, Jerzy Peisert (Wrocław, Poland)
Thermal properties of Al(110) surface – ab initio study

15. R. Sot, Jacek Piechota (Warsaw, Poland)
First principles study of selected Al twisted interfaces

16. Marian Radny (Callaghan, Australia), P.V.Smith, T.C.G. Reusch, O. Warschkow, N.A. Marks, N.J. Curson, S.R. Schofield, D.R. McKenzie, M.Y. Simmons
Charging in Atomic Resolution Scanning Tunneling Microscopy – Modelling from First Principles

17. Paweł Scharoch (Wrocław, Poland), J. Peisert
First principles thermodynamics of fcc Al crystal

18. Elwira Wachowicz (Wrocław, Poland), P. Błoński, A. Kiejna
First principles study of grain boundary impurities in iron

19. Urszula D. Wdowik (Cracow, Poland), K. Parliński
Lattice dynamics and electronic structure of Mott-Hubbard insulator from ab initio calculations

20. Martin Zelený (Brno, Czech Republic), D. Legut, M. Šob
First-principles study of magnetic phase transition in cobalt along the bcc-fcc transformation paths