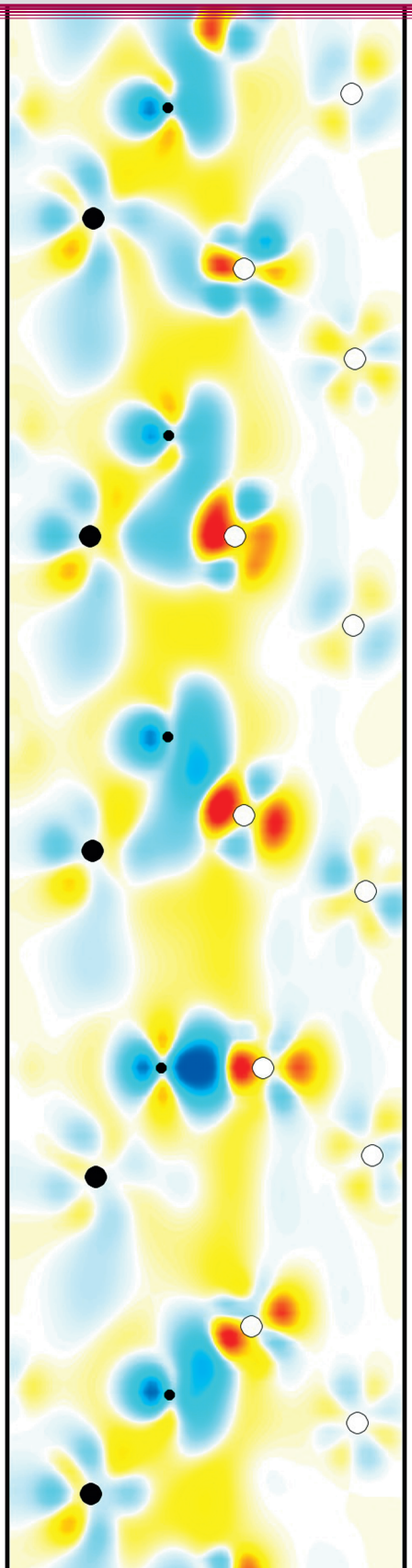
NSC News
National Supercomputer Centre at Linköpings universitet
2009:4



Real Materials are Complex

Atomic Scale Materials Theory Meets Industry

"Real materials are complex" says Göran Wahnström who performs atomic scale simulations on industrial materials.

Read further on page 3

New SNIC Landscape Document

The new SNIC Landscape Document presents several important advancements for the upcoming 4-year period.

Read further on page 2

2009 – an exciting and interesting year for NSC

The "NSC 20 years in HPC" anniversary year is approaching its end. It has been a year full of exciting and challenging events. In the middle of October, we arranged our annual international conference which was a successful event in the spirit of PRACE and future huge-scale computers (please read more about the NSC'09 conference in a separate article). An important event this year was the strategic research areas financed by the government. Of fundamental importance for NSC is of course the upcoming investments in E-science. During 2009, we have expanded our computer hall to accommodate several new systems. With the recent additions of the capacity system Kappa, available for SNAC allocations from January 2010, and the extensions of the SMHI system Gimle, we now have a total capacity of 11572 cores. Simultaneously, we have during the year recruited several persons in order to manage the increased services NSC is providing.

Now we will soon enter the year 2010 which, even if it computer-wise is not so far advanced as predicted in Arthur C. Clarke's second space odyssey, definitively will present interesting events for NSC and our users. We are expecting several new systems during the next year. We will increase our user support including assistance and collaborations on code optimisation and efficient utilisation of the NSC systems. As guidance to the close future, SNIC has recently presented the new Landscape document (cf. separate article) where the major plans for 2010–2013 are outlined.

When summing up 2009, I would like to give my deepest thanks to all devoted and knowledgeable co-workers at NSC for a prosperous year. I would also like to express our gratitude to all NSC users – we appreciate to keep regular contacts with you in order to constantly improve our services. Furthermore, I would like to thank SMHI and Saab for mutually successful partnership and our collaborators within SNIC, NDGF, EGEE, PRACE and IS-ENES for valuable cooperation. In addition, I would like to thank Linköping University for giving us faithful support.

Finally, I wish you all a Merry Christmas and a Happy New Year 2010.

BENGT PERSSON, NSC DIRECTOR

SC09 in Portland

This year, five persons from NSC went to Portland, Oregon, to take part in the SC09 conference in order to gather information on the trends of the supercomputing industry and to meet vendors and others in the field.

On the showfloor, GPU:s were still hot, with much improved double-precision performance around the corner. The OpenCL standard framework for heterogeneous computing is now available, but there was a strong dominance of NVIDIA's proprietary architecture CUDA in the posters and papers.

InfiniBand still dominated on the interconnect side, with 32 Gbps 4xQDR available, and no substantial breakthrough for 10G Ethernet compared to last year.

As you probably know, the processor vendors will be increasing the number of cores per socket during the coming years, with no significant speed-up per core in sight. The focus on energy efficiency remains high.

On the TOP500 list of supercomputers, Oak Ridge took the lead with their updated Jaguar, an Opteron-based Cray system. The Neolith cluster at NSC is still the highest-ranked Swedish academic cluster at position 104.

Portland was a nice city to visit, with better weather than predicted, a welcoming downtown district and free public transport.

KENT ENGSTRÖM

New SNIC Landscape Document

The new SNIC Landscape Document presents several important advancements for the upcoming 4-year period. The current expansion of Swedish academic computing resources needs to be accelerated even further in order to match the research requirements, with SNIC providing computing resources of different types and sizes. Thus, there is a need for increased financing, estimated to an annual total cost of 168 MSEK, excluding housing, electricity and cooling.

Already next year, SNIC plans to acquire a large capability system at one of the centres. This system should have a performance of 150–200 TFLOP/s, which is about three times faster than NSC's Neolith. In 2011, the foundation level systems ("capacity systems") should be expanded at all centres, and in 2012, Sweden will acquire its first Peta-scale capability resource.

Atomic Scale Materials Theory Meets

Quantum-mechanical atomic scale computations have become vital in materials theory. The dominating first-principles based method is the density functional theory (DFT). The combination of density-functionals, effective algorithms and high-performing computers has created a toolbox for a quantitative theory of materials. By applying these new computational tools, materials science and technology is expected to enter a new era of rapid progress and efficiency.

However, there is one major obstacle – real materials are complex. Usually they must be multifunctional, and often this can only be achieved with advanced multiphase materials, simply because different phases will uniquely contribute to the overall performance. The structure of internal boundaries or interfaces in the multiphase materials is essential for most materials properties. The arrangement of the internal surfaces, the microstructure, put huge challenges on modelling based on the atomic scale. One has to combine the atomic level description with larger length scales and, even more challenging, processes on the atomic time scale has to be connected to considerable longer time scales.

We have studied a certain class of composite materials, hard metals or more precisely WC-Co cemented carbides. These materials are produced by means of powder metallurgy, where powders of carbides and metal Co are sintered together into a hard and dense material with excellent mechanical properties. Owing to the hardness of the WC grains and the toughness of the Co binder phase, they are used as cutting and wear resistance tools and are of considerable industrial importance. The WC grains form a continuous "skeleton" of hard phase grains embedded in the metal binder phase that is also continuous. Fig. 1 shows a typical microstructure of the material with hard phase grains (red), binder phase (blue) and a huge set of grain boundaries and interphase interfaces.

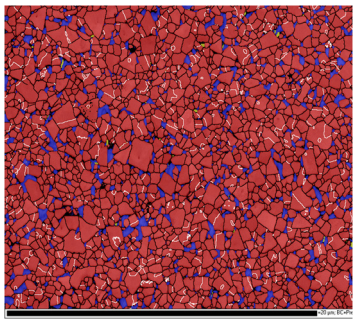


Fig. 1. A typical microstructure of WC-Co cemented carbides with WC hard phase grains (red) and Co binder phase (blue). The grain boundaries indicated with white are all so called high coincidence (sigma-2) grain boundaries. The data are obtained using the electron back-scattering technique (courtesy Mattias Elwing, Sandvik Tooling).

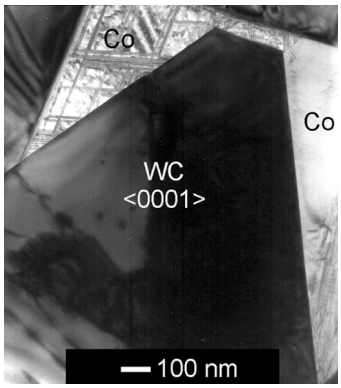
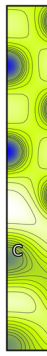


Fig. 2. WC grain in an alloy with high carbon content showing the truncated triangular form (courtesy Sabine Lay, Grenoble).

The main computational tool we have been using is the density functional theory (DFT) within a plane-wave pseudo-potential based method with projector augmented wave potentials as implemented in the Vienna ab-initio simulation package (VASP). For the exchange-correlation functional we use generalized gradient type of approximations. The program is parallelized using MPI and relies heavily on the program package BLAS for linear algebra operations. For the system sizes we are using the program scales linearly up to about 32 nodes on the NSC resource Neolith. In some cases we also perform ab-initio molecular-dynamics and we have developed and used a methodology to combine DFT data with elasticity theory to handle long range elastic effects in a correct manner [1].

The morphology, the size and shape of the WC grains is important. WC has a hexagonal geometry with an atomic arrangement that gives rise to two types of prismatic planes and one basal plane, all with either C or W termination. For the two different types of prismatic planes, type I and type II, the carbon-tungsten interplanar distance closest to the interface differs and is equal to 0.84 Å and 1.7 Å, respectively [2]. The grains are often found in the form of truncated triangular prisms (see Fig. 2) and the reason for the truncated form has been suggested to be caused by an anisotropy in the Co/WC interface energy for the two different prismatic planes.



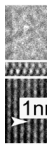
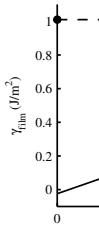
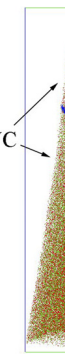


Fig. 4.
carbid





Data storage and data handling is an increasingly important SNIC activity. During 2010, the national storage SweStore will be initiated, providing cost-efficient, high-quality data storage services, also for new user communities and collaborative projects. Furthermore, the storage at each centre should be harmonised in order to make life easier for all SNIC users. In the near future, we can foresee a tremendous increase in the needs for storage, since larger and larger calculations and simulations are performed at the SNIC centres. At NSC, we already host a large part of SNIC's storage and we are happy to expand this further. On the tape storage side, procedures for cross-centre backup with off-site duplication will start during 2010, in order to increase the security even further.

Another important point in the landscape document is that SNIC now plans for an increase of application experts at the centres, providing advanced user support and help with code optimisa-

Industry

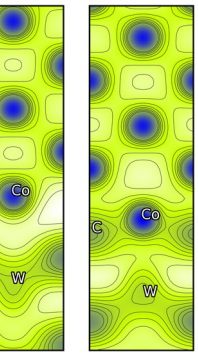
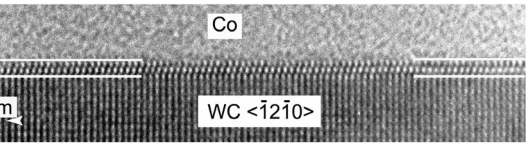


Fig. 3. The figure shows the formation of a covalent bond at a type II carbon terminated interface (to the right) as compared with the type I carbon terminated interface (to the left) as obtained from the DFT calculations.



High resolution electron microscopy (HREM) image showing a ultrathin cubic e layer lying at the WC/Co interface (courtesy Sabine Lay, Grenoble).

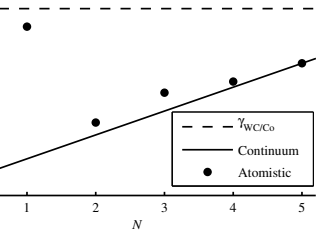


Fig. 5. Interface energy γ_{film} (J/m^2) as function of the number of layers of a cubic VC film in the WC/Co interface system. The final resulting data from the atomic scale simulations (circles) correspond to realistic doping conditions and liquid state sintering temperatures.

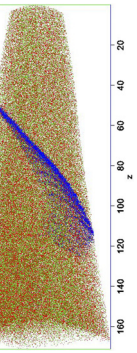


Fig. 6. Result from three dimensional atom probe field ion microscopy of a tip of WC-Co cemented carbide. The figure shows in total 2.1 million atoms (W-red, C-green, Co-blue) and the Co content in the grain boundary corresponds to about a monolayer of cobalt (courtesy Jonathan Weidow, Chalmers).

Furthermore, the shape has been shown to be effected by the carbon content (the carbon activity) during sintering. The bonding is strongly dependent on the local surrounding. In Fig. 3 we show the formation of a strong covalent bond for a type II prismatic plane. DFT calculations show indeed that the interface energy differs between the two different prismatic planes [3]. It is shown to be due to a difference in the formation of bonds with covalent character between low coordinated W and Co atoms at the prismatic planes. Quantitative agreement is obtained with the experimental determined truncation of the triangular prisms and a dependence on the carbon activity is obtained which is consistent with the experimental findings [3].

The advances of technologies for synthesis of nanosized WC and Co powders have raised the prospect of sintered nanocrystalline cemented carbides with enhanced mechanical properties. However, coarsening of nanosized particles occurs considerable more rapidly which results in fast grain growth during sintering. To retain the nanoscaled grain size has become a major challenge. One has found that by adding other carbides such as Cr_3C_2, VC, NbC, and TaC in small amounts one may mitigate the grain growth process. Especially VC has proved to be an effective inhibitor in ultrafine alloys, however, the inhibiting mechanism is not understood. Experimental high-resolution electron microscopy (HREM) studies have shown the existence of ultrathin V-rich carbide films at WC/Co interfaces in VC-doped materials at room temperature, after liquid phase sintering and cooling (see Fig 4). It has been suggested that these films hinder the grain growth by interfering with the dissolution/reprecipitation reactions at the WC/Co interface. In order to identify the grain growth inhibiting effect it then becomes decisive to determine whether these can exist at high temperature liquid phase sintering conditions where most of the grain growth occurs. At these high temperatures HREM cannot be applied. We have developed a theory for thin film formation and stability as function of temperature by combining DFT calculations for interface energies with thermodynamics modelling techniques for multicomponent systems. We find that at realistic doping conditions ultrathin films may exist at liquid sintering temperature conditions. Fig. 5 shows our computational result for the energy for an interface with a thin film as function of the film thickness. We find that an ultrathin film of two monolayers is the most stable configuration. These films, whose corresponding bulk phase is thermodynamically unstable, are stabilized by interfacial effects. Our methodology, based on theory, opens a strategy on how to control the microstructure of sintered nanocrystalline materials.

At sufficiently high temperatures and loads the material is macroscopically deformed by plastic deformation. In cutting applications this limits the cutting speed and thereby the productivity. It is found experimentally that the deformation occurs via grain boundary sliding. The continuous skeleton of carbide grains is broken up and the

tion for efficient use of the computational resources. This is completely in line with the recent extensions of services at NSC and our plans for 2010. It also goes hand in hand with the plans for SERC, Swedish E-science Research Centre, where NSC and PDC are the providers of high-performance computing resources.

There are also several changes foreseen at the international scene. EGI, European Grid Initiative, will from 2011 continue the grid services presently run within the framework of EGEE. Furthermore, several of the grid services maintained by NDGF (Nordic DataGrid Facility) will be integrated into EGI. In addition, a deepened Nordic collaboration between the national computational infrastructures is foreseen.

For further reading, you will find the SNIC Landscape document at http://www.snic.vr.se/snic-landscape-document-2010-2013

BENGT PERSSON

binder phase penetrates between hard phase grains. The driving force for this infiltration is the difference between the WC/WC grain boundary and the WC/Co interface energies. We find that most grain boundaries ought to be infiltrated by cobalt, WC/WC grain boundaries generally have a higher energy than two WC/Co phase boundaries. However, most grain boundaries are found experimentally to contain segregation of cobalt atoms, about a monolayer (cf. the figure on the front cover). We find that this segregation may decrease the grain boundary energy below that of two phase boundaries and it also increases the strength (work of separation) of the grain boundary [4]. This may explain the strength of the skeleton and it suggests a way to further strengthen the material by grain boundary engineering.

The work described here was primarily done by PhD students Mikael Christensen and Sven Johansson, but also Dan Fors, Mattias Slabanja, Sergiy Dudiy and Jan Hartford have contributed to the development of the field. We have a fruitful collaboration with experimentalists at Chalmers, Grenoble and Lausanne as well as with the companies Sandvik and SecoTools. Financial support from VR, SSF and industry is gratefully acknowledged as well as the necessary computational resources provided by SNIC.

GÖRAN WAHNSTRÖM

Front cover

WC/Co interface. The figure shows the induced electron density (blue/red- increased/decreased density) at a carbon terminated WC(0001) surface (W-large filled circles, C-small filled circles, Co- open circles).

References

[1] S. A. E. Johansson, M. Christensen, and G. Wahnström, "Interface energy of semicoherent metal-ceramic interfaces", Phys. Rev. Lett. 95, 226108 (2005).
[2] M. Christensen, G. Wahnström, S. Lay, and C. H. Allibert, "Morphology of WC grains in WC-Co alloys: Theoretical determination of grain shape", Acta Mater. 55, 1515 (2007).
[3] M. Christensen, G. Wahnström, C. H. Allibert, and S. Lay, "Quantitative analysis of WC grain shape in sintered WC-Co cemented carbides", Phys. Rev. Lett. 94, 066105 (2005).
[4] M. Christensen and G. Wahnström, "Effects of cobalt intergranular segregation on interface energetics in WC-Co", Acta Mater. 52, 2199 (2004).

Göran Wahnström is professor in Physics at Chalmers University of Technology. He has a broad interest in simulation methods in condensed matter and materials physics including electronic structure calculations, molecular dynamics and path integral simulation techniques.

NSC'09

In October NSC hosted a combined PRACE event, SNIC Interaction and 20 year celebration. The PRACE prototype system MariCel at the Barcelona Supercomputing Centre was presented as well as Anton, a specialized molecular dynamics machine from D. E. Shaw Research. We could also enjoy a description of porting and optimization work on GROMACS and a presentation of the European system for HPC applications DEISA.

The SNIC interaction part was dominated by presentations from materials science and fluid dynamics. But it was also nice to notice that scientific areas less common to HPC were represented with studies of error-correcting codes for transmissions over huge distances, experimental mathematics and laser-matter interactions in particle acceleration. Finally there was one presentation on middle ware development describing GIRD a Grid Job Management Framework.

The history of HPC in Sweden and NSC in particular was described by NSC's first director K-F Berggren. His description was complemented by presentations from NSC's partners Saab AB and SMHI as well as SUNET.

We would like to take this opportunity to thank all the speakers for their contributions.

The programme and presentations are available at http://www.nsc.liu.se/nsc09.

PETER MÜNGER

UPCOMING EVENTS

ICDCN 2010; International Conference on Distributed Computing and Networking
January 3 – 6, 2010, Kolkata, India.
http://www.icdcn.org

PPoP 2010; 15th ACM SIGPLAN Annual Symposium on Principles and Practice of Parallel Programming
January 9 – 14, 2010, Banglare, India.
http://www.ppopp.org

HPCA 2010; 16th IEEE International Symposium on High-Performance Computer Architechture
January 9 – 14, 2010, Banglare, India.
http://www.cse.psu.edu/hpcl/hpca16.html

PDP2010; 18th Euromicro International Conference on Parallel, Distributed and Network-based Processing
February 17 – 19, 2010, Pisa, Italy.
http://www.pdp2010.org

FAST'10; 8th USENIX Conference on File and Storage Technologies
February 23 – 26, 2010, San Jose, CA, USA.
http://www.usenix.org/events/fast10

Per-Com 2010; 8th IEEE International Conference on Pervasive Computing and Communications
March 29 – April 2, 2010, Mannheim, Germany.
http://www.percom.org

RAW 2010; 17th Reconfigurable Architectures Workshop
April 19 – 20, 2010, Atlanta, Georgia, USA.
http://www.ece.lsu.edu/vaidy/raw

IPDPS 2010; 24th IEEE International Parallel & Distributed Processing Symposium
April 19 – 23, 2010, Atlanta, Georgia, USA.
http://www.ipdps.org

CCGrid10; 10th IEEE International Symposium on Cluster Computing and the Grid
May 2010, Melbourne, Australia.
http://www.gridbus.org/~raj/ccgrid

PACT; 19th International Conferencon on Parallel Architectures and Compilation Techniques
September 11 – 15, 2010, Vienna, Austria.
http://www.pactconf.org

Linköpings universitet

National Supercomputer Centre, Linköpings universitet, 581 83 Linköping, Sweden
Tel: +46 (0) 13-28 26 18, fax: +46 (0) 13-28 25 35, e-mail: info@nsc.liu.se
www.nsc.liu.se

Editor: Peter Münger To subscribe, for a paper version and/or PDF-file, send an email to info@nsc.liu.se