Materials Research Cluster Gent, Room 1.16
January 31, 2013, at 10h00
Technologiepark 935, Zwijnaarde

Organised by the WOG *Computational Modelling of Materials* of the FWO-Vlaanderen

Prof. Dr. Talid R. Sinno

Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia,USA

THE ENERGY LANDSCAPE AS A TOOL FOR ANALYZING MICROSTRUCTURE IN CRYSTALS AT HIGH TEMPERATURE

Stefaan Cottenier
Center for Molecular Modeling
Ghent University
stefaan.cottenier@ugent.be

http://molmod.ugent.be

THE ENERGY LANDSCAPE AS A TOOL FOR ANALYZING MICROSTRUCTURE IN CRYSTALS AT HIGH TEMPERATURE

T. Sinno,
Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia,USA

The atomistic analysis of microstructure thermodynamics in crystalline materials at high temperature often is complicated by entropic effects that can lead to significant deviations from ground-state predictions. A common source of entropy is the presence vibrational modes associated with a particular configuration; this form of entropy is readily estimated with standard methods. More challenging to measure is the configurational entropy associated with the existence of multiple configurations. For example, a crystal defect may exhibit several degenerate (or non-degenerate) configurations that collectively lower the overall free energy of the defect. If the degeneracy is large enough, the basic thermodynamic and structural properties of a given microstructural feature can be altered significantly.

In this presentation, a theoretical-computational framework based on the notion of potential energy landscapes (PELs) and inherent structures [1,2] is developed and applied towards the thermodynamic analysis of microstructure in high temperature crystals. Briefly, the PEL represents a multidimensional map of all possible configurations in a particular system. A key feature of the PEL is the presence of numerous basins, each surrounding a local minimum energy configuration that is mechanically stable; the latter are often known as inherent structures. Under certain conditions, a system spends most of the time located near inherent structures and the PEL can be represented approximately by the collection of its inherent structures. In this study, inherent structures are found using molecular dynamics simulations coupled with energy minimization. The inherent structure energies are organized into distribution functions, which are then used for thermodynamic analysis.

We consider two primary situations. First, the physics of point defect clustering in silicon (as modeled by the EDIP potential [3]) is addressed. Defect clusters, such as nanovoids and self-interstitial precipitates, play important roles in establishing the quality of crystalline silicon for both microelectronic and photovoltaic applications. We show how entropic contributions arising from vibrational and configurational degeneracies lead to subtle but important changes in the high-temperature thermodynamics of these microstructures [4,5]. We then address the phenomenon of crystal melting in both silicon and aluminum. First, homogeneous melting in a periodic crystal is used to highlight the basic phenomenology, and then melting under more realistic conditions is considered. In particular, melting initiated at planar surfaces, at nanoparticle surfaces, and at internal cavities is compared and contrasted.

References

[1] F. H. Stillinger, and T. A. Weber, Phys. Rev. A **25**, 978 (1982).
[2] J. P. K. Doye, D. J. Wales, and M. A. Miller, J. Chem. Phys. **109**, 8143 (1998).
[3] M. Z. Bazant, E. Kaxiras, and J. F. Justo, Phys. Rev. B **56**, 8542 (1997).
[4] S. S. Kapur, M. Prasad, J. C. Crocker, and T. Sinno, Phys. Rev. B **72**, 014119 (2005).
[5] S. S. Kapur, A. M. Nieves, and T. Sinno, Phys. Rev. B **82**, (2010).
[6] A. M. Nieves and T. Sinno, J. Chem. Phys. **135**, 074504 (2011).