MM 25: Topical Session: Thermodynamics at the nano scale II - Thermodynamics

Time: Tuesday 11:45–13:00 Location: BAR 205

Topical Talk MM 25.1 Tue 11:45 BAR 205

Metal-hydrogen (M-H) systems: a tool for studying changes of thermodynamics and kinetics due to size reduction — •Astrid Pundt — Institut für Materialphysik, Universität Göttingen, Göttingen, Germany

Hydrogen easily solves on interstitial lattice sites in metals. Its high diffusivity results in short alloying times even at room temperature. At 300 K, the intrinsic defect density and the sample shape remains rather stable. This enables us to study thermodynamical and kinetical changes related to size reduction of the metal.

Many size-related effects have been reported during the last years. They are often generated by a mixture of effects due to sample size, micro-structure and mechanical stress contributions.[1] Challenge here is to split those effects related to the size reduction (finite-size effects) from those related to micro-structural changes and the mechanical stress that arises between the sample and the required stabilizer. For this, M-H thin films and M-H clusters serve as model systems. It will be shown that for systems of about 30 nm and larger the classical thermodynamics holds and conventional stress release occurs while for smaller system sizes coherent thermodynamics comes into play and ultra-high stresses are found.

Financial support by the DFG is gratefully acknowledged.

[1] A. Pundt, R. Kirchheim, Ann. Rev. Mat. Res. 36 (2006) 555.

MM 25.2 Tue 12:15 BAR 205

***Ab initio* study of AlN: thermodynamic properties, phase diagram and high temperature rock salt to wurtzite phase transition** — •Steve Schmerler and Jens Kortus — TU Bergakademie Freiberg, Institut für Theoretische Physik, Leipziger Str. 23, 09599 Freiberg, Germany

We review our recent work [1] on AlN regarding the wurtzite – rock salt phase boundary calculated within the quasiharmonic approximation by using density functional perturbation theory. We discuss exchange-correlation functional effects on the phase boundary and other thermodynamic properties. Additionally, we present *ab initio* molecular dynamics results regarding a temperature-driven rock salt to wurtzite backward phase transition and propose a detailed transition mechanism.

We would like to thank the DFG for financial support within the DFG Priority Program 1236: *Strukturen und Eigenschaften von Kristallen bei extrem hohen Drücken und Temperaturen*

[1] M. Schwarz, M. Antlauf, S. Schmerler, K. Keller, T. Schlothauer, J. Kortus, G. Heide and E. Kroke, High Pressure Res. (2013), dx.doi.org/10.1080/08957959.2013.857020

MM 25.3 Tue 12:30 BAR 205

Concept of multicomponent alloying based on self-organization on the nanoscale. — •Igor A. Abrikosov — IFM, Linköping University, Sweden

We propose a design route for the next generation of nitride alloys via a concept of multicomponent alloying based on self-organization on the nanoscale via a formation of metastable intermediate products during the spinodal decomposition. Experimentally the formation of detrimental wurtzite AlN phase has been identified as a major factor limiting the thermal stability of the state-of-the-art (TiAl)N alloys used in modern hard coating applications. We carry out systematic first-principles calculations aimed at finding potential new multicomponent transition-metal aluminum nitride alloys, and identify Cr as one of the most promising alloying elements. We predict theoretically and demonstrate experimentally that quasi-ternary (TiCrAl)N alloys decompose spinodally into (TiCr)N and (CrAl)N-rich nanometer sized regions. The spinodal decomposition results in age hardening, while the presence of Cr within the AlN phase delays the formation of a detrimental wurtzite phase leading to a substantial improvement of thermal stability compared to the quasi-binary (TiAl)N or (CrAl)N alloys [1].

[1] H. Lind, R. Forsen, B. Alling, N. Ghafoor, F. Tasnadi, M. P. Johansson, I. A. Abrikosov, and M. Oden, Appl. Phys. Lett. 99, 091903 (2011); H Lind, F Tasnadi and I A Abrikosov, New J. Phys. 15 095010 (2013)

MM 25.4 Tue 12:45 BAR 205

Reversible Phase transition of $Li_{13}Si_4$ — •Thomas Gruber and Jens Kortus — TU Bergakademie Freiberg, Institute for Theoretical Physics, Leipziger Str. 23, 09596 Freiberg, Germany

Li_xSi seems to be a promising new anode material for lithium ion batteries. For any proper application the calculation of thermodynamical data like the specific heat is required to understand the behavior of this material. There are several crystalline phase of the lithium-silicon system known and the $Li_{13}Si_4$ phase is somehow special. The phonon calculation reveal some imaginary frequencies and our evolutionary algorithm “EVO” [1] found a new similar structure. Nudged Elastic Band (NEB) method and molecular dynamic (MD) calculations were used to get a deeper insight into the phase transition between these two structures with a very low activation barrier. A very fast 1 dimensional lithium diffusion has been observed, which is very important for electrode material.

[1] S. Bahmann, J. Kortus, Computer Physics Communications 2013, 184, 1618-1625.