MM 6: Materials Design II

Time: Monday 12:00–13:00 Location: IFW D

MM 6.1 Mon 12:00 IFW D

Application of evolutionary strategies to crystal structure prediction — •Silvia Schumann and Jens Kortus — TU Bergakademie Freiberg, Institute for Theoretical Physics, Leipziger Str. 23, 09599 Freiberg, Germany

This work presents first tests of an evolution strategy for crystal structure prediction. For evaluation we chose elements of the third main group of the periodic system of elements, excluding boron. The crystal structures of these elements at ambient pressure are well known and have been selected because they have considerably different space groups, despite their same isovalent electronic structure and their similar chemistry.

For the evolution strategy a randomly chosen population of lattices is evaluated using pseudo-potentials to compute the free energy of each lattice. The more stable (lowest free energy) lattices are allowed to recombine and are mutated to form the lattices of the next generation. Contrary to conventional minimization methods the evolution strategy avoids trapping in local minima and provides a wide-range search of the high-dimensional search space. Possible slow convergence rates of evolution strategies close to minima are countered by applying conventional structure relaxation.

MM 6.2 Mon 12:15 IFW D

Structure formation described in terms of General Dynamics instead of Thermodynamics only — •Peter Häussler — Chemnitz University of Technology, Institut of Physics, 09107 Chemnitz

Phase formation is still not well understood. Generally, it is described in terms of thermodynamics under the influence of *external* parameters as e.g. volume V, temperature T, and concentration x, if alloys are described. Microscopically, by applying quantum mechanics, phase formation is described by Schrödinger's equation, dealing with *internal* quantities as the momentum $\vec{p}$, and/or angular momentum $\vec{L}$. Subsequently, till the present, there is a gap between both descriptions.

In recent contributions we were able to show that phase formation is strongly dominated by self-organizing resonances between global *internal* subsystems, causing gaps or pseudogaps at the Fermi energy of the electronic states (Peierls-, Hume-Rothery-like). The self-organization is based on an exchange of momentum and angular momentum, neither described by the present thermodynamics, nor by Schrödinger's equation as long as Bloch's theorem can not be applied (as soon the system is still without strict periodicity). We implement the internal effects between global subsystems to a description of phase formation in terms of Gibbs General Dynamics instead of Thermodynamics only. During structure formation, going from the anti-bonding resonant state to the bonding one, entropy is created, allowing the total system to release as much energy as possible.

MM 6.3 Mon 12:30 IFW D

Entwicklung einer Messmethode zur Bestimmung der Ru-Auflösung und ihrer Verifikation an einem Au/PtRu-System — •Alexander Schökel und Christina Roth — TU Darmstadt, Deutschland

Bei dem für Brennstoffzellen etablierten Katalysatorensystem PtRu kommt es im Direktmethanolbetrieb zu einer Auflösung des Ru. Dies führt zu einer Degradation der Brennstoffzelle. Untersuchungen durch Liang et al. [1] haben gezeigt, dass durch Deposition von Au-Nanopartikeln das Oxidationspotential von Ru erhöht wird und sich das Ru so gegen seine Auflösung stabilisieren lässt. Neben Au kommen auch andere Elemente für solche ternäre Katalysatorensysteme in Betracht. Theoretische Modellierungen sollen solche Kandidaten identifizieren. Katalysatorsysteme, die sich in experimentellen Untersuchungen als aussichtsreich erweisen, werden danach in Modell- und Prototypenzellen weiter untersucht.

Die TU Darmstadt entwickelt derzeit quantitative Methoden, mit deren Hilfe der Grad der Ru-Auflösung möglichst unter beschleunigten Alterungsbedingungen bestimmt werden kann. Die Entwicklung dieser Methoden und ihre Verifikation am Beispiel eines Au/PtRu-Systems sollen hier vorgestellt werden.

[1] Z.X. Liang, T.S. Zhao, J.B. Xu, J. of Power Sources 185 (2008) 166-170

MM 6.4 Mon 12:45 IFW D

Differential phase contrast setup for a non coherent beamline at HASYLAB using hard x-ray grating interferometer — •Julia Herzen[1], Felix Beckmann[1], Tilman Donath[2], Christian David[2], Franz Pfeiffer[2,3], Christian Grünzweig[2], Astrid Haibel[1], and Andreas Schreyer[1] — [1]GKSS Research Centre, Geesthacht, Germany — [2]Paul Scherrer Institute, Villigen PSI, Switzerland — [3]EPF Lausanne, Lausanne, Switzerland

Phase-contrast imaging is a common technique to visualize soft tissue with much higher contrast than the conventional absorption-contrast imaging. Differential phase contrast (DPC), developed at PSI, Switzerland, makes use of a hard x-ray grating interferometer and allows for phase-contrast imaging with high brilliance synchrotron sources as well as with conventional x-ray tubes. It is recently reported also to provide dark field information that is very sensitive to micro structures like porosity within the materials [1]. Here we present the plans to adopt the DPC technique to the HARWI-II materials science beamline [2], operated by GKSS Research Centre, in cooperation with DESY, Hamburg. This will offer an amount of new applications especially in the field of materials science like for example characterizing new light weight materials like magnesium and studying its corrosion as implant material. [1] F. Pfeiffer, M. Bech, O.Bunk, P. Kraft, E. F. Eikenberry, CH. Brönnimann, C. Grünzweig, and C. David, Nature Materials 7, pp.134-137 (2008). [2] F. Beckmann, T. Donath, J. Fischer, T. Dose, T. Lippmann, L. Lottermoser, R. V. Martins, and A. Schreyer, Proc. of SPIE Vol. 6318, 631810 (2006).