INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION

The ICAMS Seminar presents

Dr. Martin Friák
Computational Materials Design Department,
Max-Planck-Institut für Eisenforschung Düsseldorf

Monday, 19th of October, 4 p.m.
ICAMS Seminar room UHW 11/1102

Ab initio based multi-scale approaches to the elasticity of metallic polycrystals and hierarchical bio-composites

State-of-the-art *ab initio* methods constitute a solid basis of modern materials science and materials design. In order to properly address complex multi-scale phenomena that are frequently found in industrially-important materials as well as biomaterials, the theoretical research at atomistic level is increasingly combined with meso- and macro-scale approaches as well as advanced experimental techniques. Such multi-disciplinary modeling strategies will be exemplified by a scale-bridging approach to the integral elastic response of (i) multi-phase metallic polycrystals and (ii) biomaterials with hierarchical microstructure. Both topics combine (i) single crystal thermodynamic and elastic stiffness data determined by parameter-free first-principles calculations and (ii) case-specific homogenization schemes. Due to the fact that the mathematical backbone of our coarse-graining approach could be non-linear, its error-propagation properties have been investigated and the dependence of the final output parameters on the scale-transferred ab initio input data is shown. The reliability and error-bars of the methodology are cross-validated against the experimental data for a few selected systems, specifically (i) Ti-Nb alloys intended for medical applications [1], (ii) ultra light-weight Mg-Li alloys [2], and (iii) hierarchical chitin-based biocomposites [3].

Literature

1. D. Raabe, B. Sander, M. Friák, D. Ma, and J. Neugebauer: Theory-guided bottom-up design of β-titanium alloys as biomaterials based on first principles calculations: Theory and experiments, Acta Materialia 55, 4475 (2007).
2. W. A. Counts, M. Friák, D. Raabe, and J. Neugebauer: Using ab initio calculations in designing bcc Mg-Li alloys for ultra light-weight applications; Acta Materialia 57, 69 (2009).
3. S. Nikolov, C. Sachs, H. Fabritius, D. Raabe, M. Petrov, M. Friák, J. Neugebauer, L. Lymperakis, and D. Ma: Hierarchical modeling of the mechanical properties of lobster cuticle from nano- up to macroscale: The influence of the mineral content and the microstructure; Advanced Materials, accepted (2009).