Spring 2018 Joint Colloquium
Materials Department & Materials Research Laboratory

Professor Bob Svendsen

Chair of Material Mechanics
Division of Material Science and Engineering
Dept. of Georesources and Material Engineering
RWTH Aachen University

Dept. of Microstructure Physics and Alloy Design
Max-Planck-Institut für Eisenforschung GmbH

Friday, April 20th, 2018
11:00 am, ESB 1001

Phase-field Chemomechanical Modeling of Nanoscopic Dislocation-precipitate Interaction in Metallic Alloys

The purpose of the current work is the development and application of continuum thermodynamic models for the effect of solute chemistry and segregation on dislocation-mediated deformation in metallic alloy systems at the nanoscopic scale. Examples of such systems include two-phase - γ–γ' nickel-based superalloys or two-phase γ-κ high maganese lightweight steels. Model development is carried out in the framework of a recent phase-field-based approach to the formulation of chemomechanics for multiphase, multicomponent solid systems [3]. In this framework, models for dislocation-solute and -microstructure interaction build in particular on *ab initio*- and atomistics-based Peierls-Nabarro and phase-field models for nanoscopic dislocation processes (e.g., dissociation, core and stacking fault formation) in single-element fcc materials [e.g., 1, 2, 6]. Basic aspects of the extension and generalization of these models to multicomponent, multiphase alloy systems will be discussed, e.g., the effect of solutes on the (generalized) stacking fault energy. In addition, initial simulation results for dislocation-precipitate interaction in Ni-Al alloys will be presented and compared with analogous MD simulation results as well as with related previous work [e.g., 4, 5, 7]. If time permits, preliminary results for the Ni-Al-Co system will also be discussed.

[1] Hunter, A., Zhang, R. F., Beyerlein, I. J., Germann, T. C., Koslowski, M., 2013. Dependence of equilibrium stacking fault width in fcc metals on the gamma-surface. Modelling and Simulation in Materials Science and Engineering 21, 025015 (19pp).

[2] Mianroodi, J. R., Hunter, A., Beyerlein, I., Svendsen, B., 2016. Theoretical and computational comparison of models for dislocation dissociation and stacking fault / core formation in fcc crystals. Journal of the Mechanics and Physics of Solids 95, 719–741.

[3] Svendsen, B., Shanthraj, P., Raabe, D., 2018. Finite-deformation phase-field chemomechanics for multiphase, multicomponent solids. Journal of the Mechanics and Physics of Solids 112, 619–636.

[4] Vorontsov, V. A., Shen, C., Wang, Y., Dye, D., Rae, C. M. F., 2010. Shearing of γ' precipitates by a(112) dislocation ribbons in Ni-base superalloys: a phase field approach. Acta Materialia 58, 4110–4119.

[5] Vorontsov, V. A., Shen, C., Wang, Y., Dye, D., Rae, C. M. F., 2012. Shearing of γ' precipitates in Ni-base superalloys: a phase-field study incorporating the effective γ-surface. Philosophical Magazine 92, 608–634.

[6] Wang, Y., Li, J., 2010. Phase field modeling of defects and deformation. Acta Materialia 58, 1212–1235.

[7] Zhou, N., Shen, C., Mills, M. J., Li, J., Wang, Y., 2011. Modeling displacivediffusional coupled dislocation shearing of γ precipitates in Ni-base superalloys. Acta Materialia 59, 3484–3497.

Bio

Degrees. 1980: B.Sc., Geological Sciences, Bradley University, Peoria, Illinois. 1982: M.Sc., Geophysics, Caltech. 1987: Ph.D., Geophysics and Applied Physics, Caltech. 1992: Habilitation (second Ph.D., Geman system), Theoretical and Applied Mechanics, Technical University of Darmstadt, Germany. **Positions.** 1987-1988: Postdoc, Geophysics, Swiss Federal Institute of Technology (ETH), Zurich, Switzerland. 1989-1994: Lecturer, Theoretical and Applied Mechanics, Technical University of Darmstadt, Germany. 1995-1999: Research Fellow, Federal Institute for Materials Research and Testing (BAM), Berlin, Germany. 2000-2010: Full Professor, Engineering Mechanics, Technical University of Dortmund, Germany. Since 2010: Research Professor, Material Mechanics, Division of Material Science and Engineering, RWTH Aachen University, Aachen, Germany. Since 2011: Senior Scientist, Microstructure Physics and Alloy Design, Max-Planck-Institut fur Eisenforschung, Dusseldorf, Germany. **Publications.** Available at ResearchGate (www.researchgate.net), Researcher ID (www. researcherid.com/rid/D-6311-2014), Orcid ID:orcid.org/0000-0002-1519-9433.

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Hosted by Irene Beyerlein.