

MM 18: Invited talk Stukowski

Time: Tuesday 9:30–10:00

Location: TC 006

Invited Talk MM 18.1 Tue 9:30 TC 006
Unraveling the Mechanisms of Plasticity in Nanostructured Materials using Advanced Data Analysis and Simulation Methods — ●ALEXANDER STUKOWSKI — Institut für Materialwissenschaft, TU Darmstadt

Nanocrystalline, nanotwinned, and nanoporous metals and alloys all exhibit exceptional deformation behavior due to their large density of internal interfaces. Unlike in more coarse-structured materials, a multitude of mechanisms contributes to the plasticity and strength of these novel materials, leading to more complex mechanical behavior.

Large-scale molecular dynamics and new Monte-Carlo simulation methods [1] possess the potential to significantly expand our understanding of the underlying processes that govern the plasticity at the

nanoscale. In particular the recent development of sophisticated data analysis algorithms [2] helps us to identify, track, and visualize key microstructural features and defects in complex materials models, leading to new insights into the interplay of competing mechanisms [3] and the internal evolution of materials.

I will highlight several of our recent developments in this active field of research, demonstrate the power of these enabling technologies by looking at different materials systems [4], and discuss challenges yet to be solved in this area of computational materials science.

[1] B. Sadigh et al., Phys. Rev. B 85 (2012), 184203

[2] A. Stukowski, JOM 66, Issue 3 (2014), 399-407

[3] J. Schäfer et al., J. Appl. Phys. 114 (2013), 143501

[4] A. Stukowski, K. Albe, D. Farkas, Phys. Rev. B 82 (2010), 224103