



TECHNISCHE UNIVERSITÄT
CHEMNITZ

Institut für Physik Physikalisches Kolloquium



Mittwoch, 27.04.2016, um 16:00 Uhr

Ort: Reichenhainer Str. 90;
Zentrales Hörsaal- und Seminargebäude,
Raum 2/N013

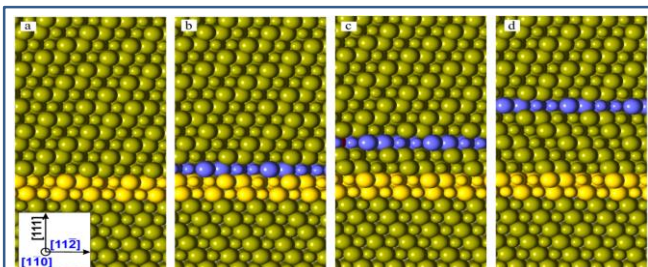
Dr. Rebecca Janisch

Ruhr-Universität Bochum
ICAMS

Grain boundary properties from atomistic simulations and their use in mechanical modelling of materials

Modern structural materials are seldom single crystals, but exhibit a polycrystalline, multiphase, often hierarchical microstructure. Consequently, "there is not one material property that is unaffected by the presence or absence of grain boundaries." (A.D. Smith 1996), and the effect of interfaces on the mechanical properties of materials is in fact manifold.

Nowadays tailored microstructures, containing certain arrangements of grain boundaries with specific properties that can even be tuned by segregation engineering, are within experimental reach. This gives additional impetus to the development of predictive material models that bridge between the atomistic details of grain boundaries and the effective properties of the microstructure, and can



Snapshots of a molecular dynamics simulation of bicrystal shear in TiAl. A stacking fault (blue atoms) is emitted from the interface (yellow atoms).

help to identify microstructures with optimized mechanical properties. Numerical simulation methods, that either allow the study of relevant processes on their characteristic length scale, or can be used to pass on information from finer to coarser length scales, are common tools in this respect. In the presentation some examples of atomistic studies of grain boundaries will be given that illustrate current developments and the challenges that one has

to face when trying to extract effective mechanical behavior and to link it to fundamental physical and geometrical properties of the interfaces.

Alle Zuhörer sind ab 15:45 zu Kaffee und Tee vor dem Hörsaal eingeladen.

Informationen zum Vortrag erteilt:

Prof. Dr. Michael Schreiber, Tel. 0371 531-21910



www.tu-chemnitz.de/physik