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EINLADUNG

zum Gastvortrag

von

Dr. Vikas Tomar

Purdue University, West Lafayette-IN, USA

am

Dienstag, 10.06.2014, 11.00 (c.t.) Uhr

Technische Universität Wien, Karlsplatz 13, 1040 Wien
Sem 202 (Stiege 2, 2. Obergeschoß + Halbstock)

A NANOMECHANICS BASED INVESTIGATION INTO INTERFACE DEFORMATION IN A SET OF INORGANIC AND ORGANIC MATERIALS

From the biological/chemical perspective, interface concepts related to cell surface-synthetic biomaterial interface and extracellular matrix-biomolecule interface have wide applications in medical and biological/biomaterial technology advancements. From inorganic materials (metals/alloys/ceramics) perspective, interfaces and grain boundaries hold significant promise in terms of controlling and engineering material properties as a function of environment, temperature, and different types of loading conditions. In this talk, a brief overview of recent advances made in my group regarding grain boundary and interface property dependent properties of metals, ceramics, and biomaterials is presented. First problem of focus is grain boundary embrittlement in high temperature/refractory metals. A multiscale analysis based strategy that uses thermomechanical and grain boundary thickness dependent properties using quantum mechanical *ab-initio* simulations is used to predict microstructure dependent grain boundary embrittlement in materials. A scaling model that takes into account chemical properties of grain boundaries to predict grain boundary embrittlement dependent fracture in materials is described. Analyses establish a notion that its not only the mechanical (stress-strain) but thermal (phononic and electronic properties) properties too that govern chemical structure dependent deformation properties of material interfaces. Such a notion is found to guide behavior of interfaces in a high temperature ceramic as well. Finally, such a notion is extended to biomaterial interface properties including a prediction of correlation between thermal properties of biological interfaces with the deformation dependent interface stresses and interface viscosity. More importantly, interface topology and roughness are indicated to play an important role in hierarchy dependent properties of biological materials. Based on these observations, some biomimetic material design principles are analyzed.

BRIEF BIOGRAPHY:

Dr. Vikas Tomar is an Associate Professor in the School of Aeronautics and Astronautics at Purdue University. He obtained his Ph.D. from Georgia Tech in Dec. 2005. Dr. Vikas Tomar works in the area of multiscale simulations and experimentation of material failure with an account of interface, grain, and grain boundary level properties. His particular emphasis is on predicting and analyzing material failure in extreme environments, where he has made contributions using a combination of multiscale models with multiscale experiments. Dr. Tomar has developed a new experimental paradigm based on nanomechanical and micromechanical Raman spectroscopy (Published in Journal of Engineering Materials and Technology and Materials Science and Engineering-A, 2010-11, AIP Review of Scientific Instruments, 2014). In these experiments *in-situ* simultaneous measurements of nanoscale and mesoscale thermal and mechanical properties in a material can be performed while the structure is being loaded *ex-situ*. The simulation methods developed in his group include: (a) a new non-equilibrium Green's function (NEGF) based formalism to understand the influence of high temperature and extreme environment assisted phase transformation in nanostructured materials (published in J. Europ. Ceram. Soc. 2012 and J applied Physics 2013), (b) a new variant of the cohesive finite element method (CFEM) to analyze microscale failure in composites with an account of stochasticity in material properties (Engineering Fracture Mechanics, 2005); and (c) two different variants of molecular simulation methods (published in Journal of Applied Physics, Physica Status Solidi-a) for speeding up non-equilibrium molecular simulation timescales. He has used such advances to analyze microstructure dependent failure of materials where material properties in materials can be specified with an account of nanoscale to micron scale microstructure feature properties (e.g. a grain boundary or a grain undergoing phase transformation or uncertainty in material or microstructure representation). Overall, Dr. Tomar has written over 100 articles including 70 international journal publications. He has won multiple research awards in US including from ASME, Elsevier, TMS, and AFoSR. He is also currently an Editor-In-Chief of International Journal of Experimental and Computational Biomechanics and Journals of Materials-Nanoscience.