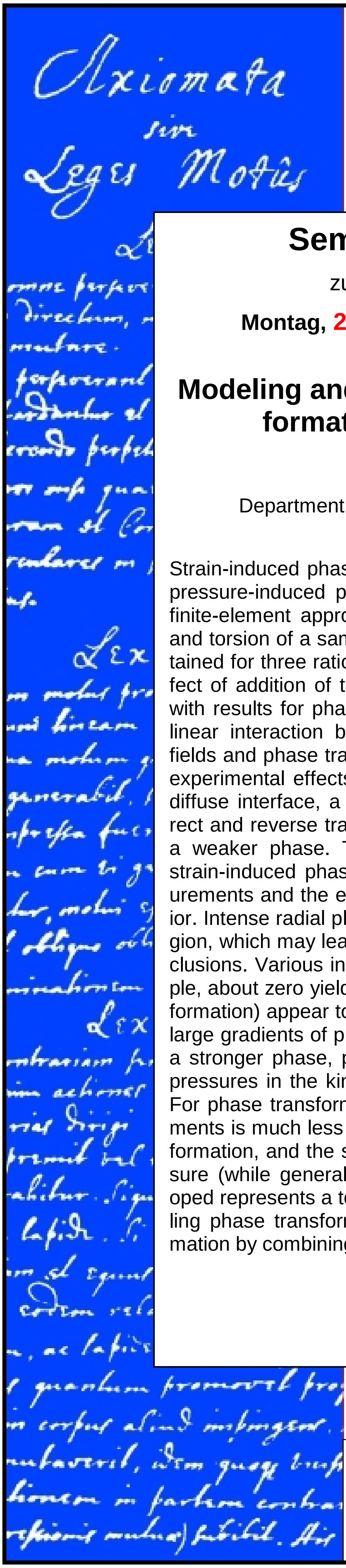

Friedrich-Alexander-Universität
Erlangen-Nürnberg

Seminar über Fragen der Mechanik

zu folgendem Vortrag wird herzlich eingeladen

Montag, 21.05.2012, 14:00 Uhr, Egerlandstr. 5, Raum 0.044

Modeling and Simulation of Strain-Induced Phase Transformations in Rotational Diamond Anvil Cell

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Strain-induced phase transformations under high pressure differ significantly from the pressure-induced phase transformations under hydrostatic conditions. A model and finite-element approach to strain-induced phase transformations under compression and torsion of a sample in rotational diamond anvil cell are developed. Results are obtained for three ratios of yield strengths of low-pressure and high-pressure phases. Effect of addition of torsion on phase transformation process is studied and compared with results for phase transformation under compression only. A very nontrivial, nonlinear interaction between strongly heterogeneous stress and plastic strain tensor fields and phase transformation kinetics is revealed, quantified, and analyzed. Various experimental effects are reproduced, including plateau at pressure distribution at the diffuse interface, a pressure self-multiplication effect, simultaneous occurrence of direct and reverse transformations, and irregular stress distribution for transformation to a weaker phase. The obtained results change the fundamental understanding of strain-induced phase transformation in terms of interpretation of experimental measurements and the extracting of information on material processes from sample behavior. Intense radial plastic flow moves the high-pressure phase into the low-pressure region, which may lead to misinterpretation of measurements and to drawing wrong conclusions. Various interpretations based on a simplified equilibrium equation (for example, about zero yield strength of phase mixture and hydrostatic conditions during transformation) appear to be wrong because of inapplicability of this equation for cases with large gradients of phase concentration and yield strength. For phase transformation to a stronger phase, pressure at the diffuse interface corresponds to the characteristic pressures in the kinetic equation, which allows us to determine them experimentally. For phase transformation to a weaker phase, this is not true, and analysis of experiments is much less robust. In fact, for this case torsion does not promote phase transformation, and the statement that plastic straining reduces phase transformation pressure (while generally correct) was not experimentally justified. The approach developed represents a tool for designing experiments for different purposes and for controlling phase transformations, and it opens unexpected ways to extract material information by combining simulation and experiment.

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