INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION

Special Seminar

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ICAMS Seminar room UHW 11/1102

Investigation of the defect structure of nanoparticles during mechanical stressing

It has been shown that by wet grinding in stirred media mills, the production of particles with sizes of 10 nm is possible. Fracture mechanisms on the nanometer scale are not yet understood and are subject of current investigations. Analyses of samples from milling experiments with high resolution transmission electron microscopy yielded several interesting microstructural details. It was found that samples of SnO_2 particles featured shear bands and crystal twins while the CaF_2 particles contained dislocations. Molecular Dynamics simulations were conducted with the goal of describing the influence of microstructure and size dependent material properties on the fracture behaviour of SnO_2 and CaF_2 nanoparticles. Spherical particles of up to 30 nm were compressed uniaxially between two milling beads. The produced microstructures showed a remarkable agreement with the experimental results. Like in the experiments, the lattice of the SnO_2 particle was dominated by shear bands and crystal twins stemming from plastic deformation. The CaF_2 nanoparticles also deformed plastically but through the motion of dislocations. A limited stability of these dislocations was observed upon stress release. Also size effects were found for the elastic behaviour of the particles and the density of defects.