Institut für Numerische Simulation
Rheinische Friedrich-Wilhems-Universität Bonn

hausdorff center for mathematics

Einladung zu einem Vortrag im Seminar Materialwissenschaften und Mathematik

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spricht zum Thema

Atomistic insights into the tribological and rheological properties of carbon nanomaterials

Zeit: **Donnerstag, den 07. Juli 2011, 16:00 Uhr**
Ort: **Endenicher Allee 60, Seminarraum 2.040**

gez. **Prof. Dr. Michael Griebel, Prof. Dr. Stefan Müller**

Abstract: Often a computer-aided understanding and design of nanomaterials and processes relies on classical molecular dynamics. Too often however, such atomistic simulations are limited by the accessible time and length scales. In this lecture, the atomistic/continuum multiscale coupling is used to overcome these limitations: classical molecular dynamics simulations on small time and length scales are used to derive nanoscale continuum equations that quantitatively reproduce the atomic scale processes. Often these continuum equations include novel terms that are required to describe finite size effects of the considered systems. Using the decay of propane nanojets, nano capillary impregnation, growth of carbon nanotubes and diamond-like carbon as well as wear in diamond, it will be demonstrated that atomistic/continuum multiscale coupling represents a useful strategy tounderstand and describe unique nanoscale processes, such as finite size pressure fluctuations in capillary systems, the role of slip boundaries in impregnation processes, surface diffusion mediated dynamics of catalyst particles in carbon nanotubes and the deposition of self-smoothing diamond-like carbon nanofilm growth. At the end of the lecture, a six century old riddle will be solved [1].

[1] Lars Pastewka, Stefan Moser, Peter Gumbsch, Michael Moseler, Anisotropic mechanical amorphisation drives wear in diamond *Nature Materials* 10, 34 (2011)