

## Mechanik-Seminar

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- Referent: **Prof. Gerard L. Vignoles**  
LCTS - Lab for ThermoStructural Composites, Pessac, France
- Datum: Donnerstag, 05.05.2011  
Uhrzeit: 15:45-17:15 Uhr  
Ort: Geb. 10.23, 1. OG, SR 1, R 104
- Thema: **"Modelling structure and properties of pyrocarbons from image-guided atomic-scale reconstructions"**  
(Struktur- und Eigenschaften-Modellierung von Pyro-Kohlenstoffe aus bildgeleiteten atomischen Rekonstruktionen)
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**Abstract:** This talk will introduce an original approach for the construction of atomic scale models for nanotextured materials such as pyrocarbons based on HRTEM lattice fringe imaging. Starting from an HRTEM LF micrograph with high- and low-frequency filtering, a set of 2D image statistical descriptors is collected. This set is imposed as a constraint to a random 3D image generator with a transverse isotropy hypothesis. The generated 3D images are then used as an attractive potential field superimposed to the usual intermolecular potentials in Molecular Dynamics simulations of liquid carbon quenching. The obtained set of up to 20,000 carbon and hydrogen atoms may be used for the evaluation of several properties. First, structural properties like simulated HRTEM LF images and pair distribution functions are compared to experimental data, with an excellent agreement. Second, a virtual mechanical testing of the structure is presented and discussed.

References: J.-M. LEYSSALE, J.-P. DA COSTA, C. GERMAIN, P. WEISBECKER, and G. L. VIGNOLES, Appl. Phys. Lett. (2009), vol. 95, 231912

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**Alle Interessenten sind herzlich eingeladen!**

Prof. Dr.-Ing. Thomas Böhlke