# MM 57: Invited talk Markmann

Time: Thursday 15:00–15:30 Location: H38

**Invited Talk** MM 57.1 Thu 15:00 H38

**Virtual diffraction as a tool to investigate nanostructured materials** — •Jürgen Markmann — Helmholtz-Zentrum Geesthacht, Institut für Werkstoffforschung, Werkstoffmechanik, Geesthacht, Germany — Technische Universität Hamburg-Harburg, Institut für Werkstoffphysik und Werkstofftechnologie, Hamburg, Germany

The boost in computational resources during the last years caused a considerable increase in simulation studies of materials on the atomistic scale. Several tools for detailed local analyses have been developed but they usually leave the difficulty of transferring the gained knowledge into macroscopically measurable data. Knowing the exact position of the mass centres (atoms or grid points) of a material allows the calculation of its wide-angle and small-angle diffraction pattern. Taking into account all experimental artefacts, these virtual diffraction patterns can be analysed in an identical way one would do it in a laboratory experiment. A modification of the method also makes direction dependent investigations possible. Shown here are findings revealed by application of this method on MD simulated nanocrystalline palladium during deformation and the first tries to apply this method to nanoporous gold. Among other things, an intrinsic nature of microstrain in nanocrystalline materials was discovered and the contribution of grain boundaries to the elastic deformation of nanocrystalline materials was illustrated.

[1] Markmann, Yamakov, Weissmüller, *Scripta Mater.* **59** (2008) 15.
[2] Markmann, Bachurin, Shao, Gumbsch, Weissmüller, *Europhys. Lett.* **89** (2010) 66002.