

## **DFG Research Group: Plasticity in Nanocrystalline Metals and Alloys:**

The research group was established in July 2006 with 5 projects working experimentally and theoretically on the plasticity of nanocrystalline Pd and Pd alloys. The group is represented by the spokesman, Dr. Jörg Weissmüller (INT, Forschungszentrum Karlsruhe), and the deputy spokesman, Prof. Oliver Kraft (izbs). The central office of the group for organizational and administrative duties is located at izbs.

### **Project 2: Molecular dynamics simulation of deformation of nanocrystalline palladium**

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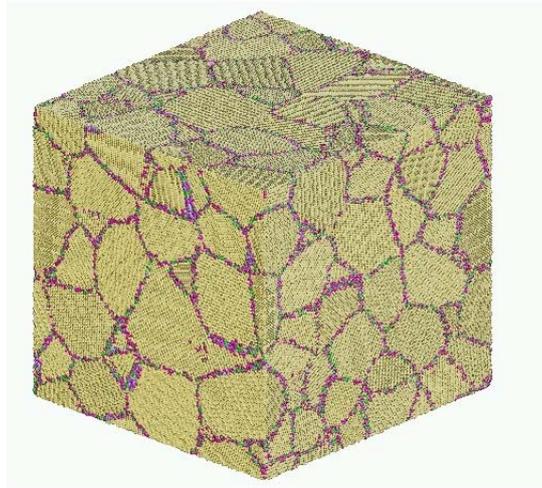
The deformation mechanisms of nanocrystalline metals are far from being well understood. Dislocation sources are lacking within small grains, therefore either grain boundaries act as sources and sinks for dislocations, or intragranular deformation caused by grain boundary sliding, grain boundary migration, grain rotation and diffusion processes takes place; often both mechanisms contribute to the deformation of nanocrystalline materials.

One of the important questions is how the grain size of materials influences the observed deformation mechanism. Recent molecular dynamics simulations in 3D nickel samples have shown an increased (partial) dislocation activity when the grain size increased from 12 to 20 nm and no dislocation activity for grain sizes of 5 nm. Thus, reducing the grain size leads to an activation of intragranular deformation mechanisms, whereas the increase of the grain size is followed by a gradual increase in the role of intragranular deformation caused primarily by the motion of dislocations.

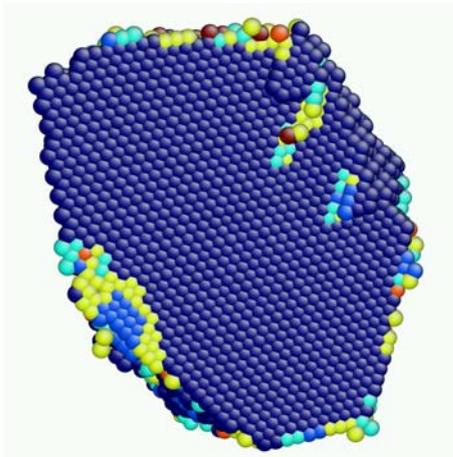
An Embedded Atom Method potential for palladium is used to study deformation mechanisms in nanocrystalline structures that have previously been investigated for aluminum. The 3D sample containing 100 randomly oriented grains with mean grain size of 10 nm were taken as initial structure (see Fig. 1). The sample was first relaxed, annealed and then equilibrated at room temperature and at zero external pressure. Grain sizes are distributed from 6 to 16 nm and grain boundary misorientations are random. A uniaxial tensile strain with different strain rates was applied to the sample. All simulations were performed at room temperature.

Extended partial dislocations are expected during deformation as in similar investigations on Al or Ni. Simulations however, reveal that palladium responds to the loading by fracturing grain boundaries at uniaxial strain of approximately 3%. The cracks are nucleated on grain boundaries which are oriented perpendicular to the applied strain. Such brittle behavior of nanocrystalline palladium is also found in experimental investigations.

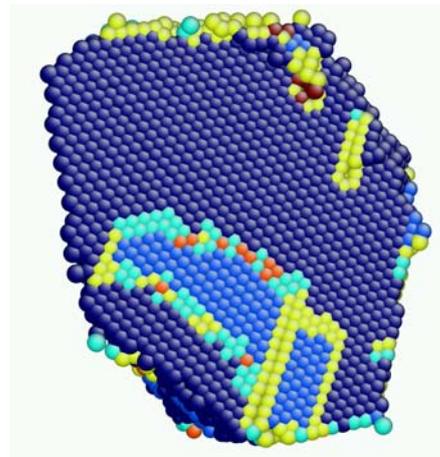
No partial or full dislocation passed through an entire grain up to 3% of strain. However, several dislocation embryos exist near grain boundaries. These nucleated dislocations are strongly pinned and cannot break away from the grain boundaries even at high applied strain. A few of the embryos are jogged full dislocations, where the segments of the dislocation lines are not in one glide plane, but extend over more than one interplanar spacing (see Fig. 2). In spite of the grain size distribution, no increased dislocation activity was found, even in the largest grains of the sample. Therefore, one can conclude that the stresses necessary for depinning the dislocation embryos in nanocrystalline palladium are probably smaller than the stresses required for crack opening. Dislocation configurations and the first fracture events will be investigated further.



**Fig. 1:** Computer-simulated sample of nanocrystalline palladium with periodic boundary conditions in all directions. Each side of the box is 41 nm long and the sample contains 4.6 million atoms. Yellow atoms correspond to an ideal fcc crystal lattice; other colored atoms are grain boundary atoms



(a)



(b)

**Fig. 2:** A view of the nucleation of the full dislocation followed by a nucleation of the partial dislocation located one slip plane below and their partial transmission into the grain interior. (a) initial (undeformed) configuration; (b) after 3% of strain. Atoms are colored according to their local crystalline order