

NOVEL DEFORMATION PROCESSES DOMINATE AT THE NANOSCALE

SCIENTIFIC ACHIEVEMENT

Large-scale atomic-level simulations revealed how and why conventional dislocation deformation processes break down at the nanoscale, i.e., for a grain size of typically below 30 nm. These simulations demonstrated that, as the grain size becomes ever smaller, a material becomes ever harder to deform, which is consistent with observed behavior. At a certain point, dislocations cannot exist at all anymore because their size becomes comparable to that of the grains themselves. At this critical size, the material suddenly softens again due to the onset of novel deformation mechanisms controlled by the grain boundaries. Our simulations revealed that this “strongest size” is a function of not only the material itself but also the stress level to which it is subjected. Our simulations also revealed the extensive occurrence of deformation twinning for the larger grain sizes (i.e., above the “strongest size”). This mechanism is usually thought to be operational only in coarse-grained polycrystals. However, stimulated by our prediction of deformation twinning as an important deformation mechanism particularly in nanocrystalline materials, experiments performed on Al have recently observed the existence of this important deformation process. Based on these observations, it is now thought that the strengthening of these materials with decreasing grain size may not be due to dislocation pile-ups but, instead, due to the obstacles for moving dislocations represented by these twins.

SIGNIFICANCE

Functional nanostructures can experience very high internal stress levels resulting either from their very functionality or induced by thermo-mechanical processing; mechanical stability and compliance therefore represent major obstacles in the development of nanodevices. The insights gained from these simulations will enable the design of nanodevices with tailored mechanical performance. In addition, they will lead to mechanically optimized functional nanostructures capable of withstanding the very high stresses under which they often operate.

REFERENCES

Dislocation processes in the deformation of nanocrystalline aluminum by molecular-dynamics simulation, V. Yamakov, D. Wolf, S. R. Phillpot, A. K. Mukherjee and H. Gleiter, *Nature Materials* **1**, 1-4 (2002).

Length-scale Effects in the Nucleation of Extended Dislocations in Nanocrystalline Al by Molecular-Dynamics Simulation, V. Yamakov, D. Wolf, M. Salazar, S. R. Phillpot and H. Gleiter, *Acta Mater.* **49**, 2713-22 (2001).

Deformation twinning in nanocrystalline Al by molecular-dynamics simulation, V. Yamakov, D. Wolf, S. R. Phillpot and H. Gleiter, *Acta Mater.* **50**, 5005-20 (2002).

PERFORMERS

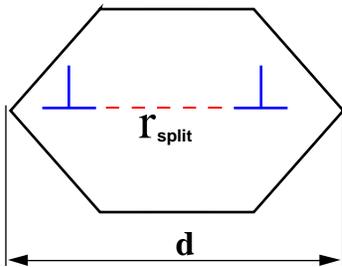
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Novel Deformation Processes Dominate at the Nanoscale

Crossover from dislocation to grain-boundary plasticity with decreasing grain size:

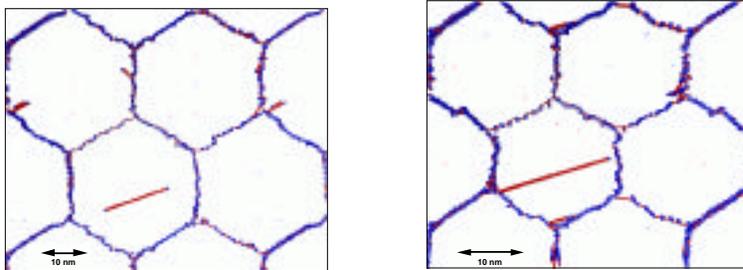
- Size of a Frank-Read source cannot exceed grain size, d : i.e., for a nm grain size, these sources are not operational!
- However, dislocations can then be nucleated from the GBs.
- Dislocation splitting rapidly increases with applied stress, σ .



$$r_{\text{split}} = Kb^2/(\Gamma_i - bm\sigma)$$

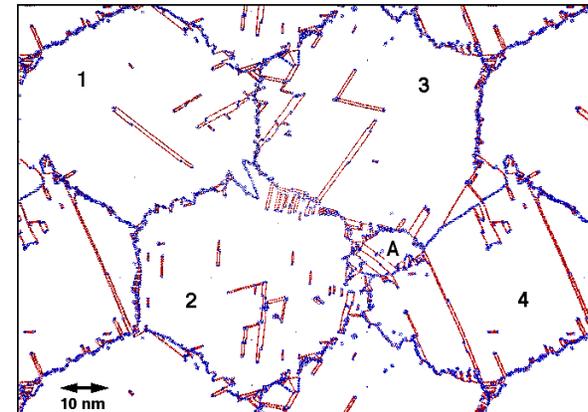
Γ_i = stacking-fault energy

Why the dislocation-slip mechanism shuts down for small grain size



Snapshots for a grain size of 30 nm (left) and 20 nm (right) after ~1% tensile deformation in the horizontal direction at 300 K. Whereas for the larger grain size a complete extended dislocation is emitted from the grain boundary on the left, for the smaller grain size complete emission is no longer possible.

Deformation substructure, including twinning at the nanoscale



Snapshot of a <110> textured Al polycrystal with a grain size of 45 nm at 11.9% plastic strain. A variety of processes involving dislocation-dislocation and dislocation-GB interactions has taken place, including deformation twinning. Following our prediction, deformation twinning in nanocrystalline Al has recently been observed experimentally.

Summary:

- Two length scales in dislocation nucleation from the grain boundaries: r_{split} and d !
- for $d = r_{\text{split}}$, dislocation slip mechanism ceases to operate
- Crossover to deformation via grain-boundary sliding

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