Atomic-level Mechanisms of Grain Boundary Migration

Scientific Achievement

In collaboration with the Max-Planck-Institut in Stuttgart, Germany, researchers at Argonne National Laboratory have been able to perform atomic-level studies of the dynamics of grain boundary (GB) motion at elevated temperature. Through novel thin film specimen preparation techniques it was possible to observe the real-time temporal behavior of grain boundaries by high-resolution transmission electron microscopy (HREM). In this manner previously unexplored atomic processes at elevated temperature have become accessible to atomic-level analysis.

Thin bicrystalline films of gold and aluminum are grown using novel epitaxial templating techniques developed at Argonne. This process includes deposition of high-purity materials and control of grain misorientation. Nanoscale island grains allow HREM observation of all low-energy facets at a given in-plane misorientation. Tilt grain boundaries as well as general GBs, i. e. grain boundaries with tilt and twist components could be observed at high temperature in the atomic-resolution HREM at the MPI in Stuttgart, Germany. Video recordings of GB migration were digitally analysed to allow precise comparison of nano-scale areas as a function of time with a temporal resolution of 1/30 s.

As a function of GB geometry, three primary GB migration mechanisms were elucidated at the atomic level: glide, ledge mechanisms, and cooperative shuffles. In high-angle GBs, including tilt as well as general GBs the most common mode of thermally activated GB migration included cooperative atomic shuffles, with temporally highly varying speeds of GB propagation. Curvature as as well as surface energy driven GB migration was demonstrated. For the first time, direct evidence for the existence of collective effects in GB migration was obtained from a study of spatial fluctuations of GB position at high temperature. In the absence of a driving force for migration certain nano-size regions at grain boundaries, typically involving up to several hundred atoms, were found to switch back and forth between neighboring grains. Such reversible structural fluctuations were found in [110] and [001] tilt, as well as a general grain boundary. The existence of rapid atomic shuffles that can accomplish the necessary lattice rotations between neighboring grains was directly demonstrated by these observations.

Significance

Most materials are polycrystalline, i. e. they consist of many crystalline regions. The boundaries between these grains have a relatively high energy. At high enough temperatures these boundaries migrate in order to reduce their total energy, thus changing the grain size and structure. Grain boundaries determine many important properties of crystalline materials, including strength and toughness, corrosion resistance, and electrical properties. Achieving desired materials properties involves controlling the effect of grain boundary motion on microstructure. An understanding of the atomic mechanisms of grain boundary motion is therefore of key importance in achieving improved material properties.

Performers:

K. L. Merkle, L. J. Thompson, F. Phillipp (MPI Stuttgart) Philos. Mag. Lett. 82, 589 (2002).
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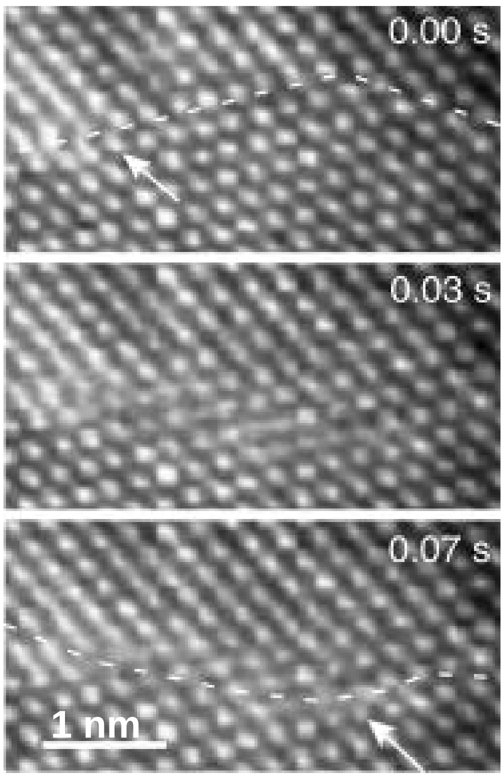

Au [110], θ =50°, 710 °C.

Atomic-resolution movies of crystalline lattices near grain boundaries are obtained at high temperature by in-situ high-resolution transmission electron microscopy.

The results show rapid back-and-forth movements of the grain boundary at high temperature.

This indicates that cooperative atomic shuffles whose individual movements are small, but involve hundreds of atoms, can rapidly advance a grain towards its neighbor.

Results are of key importance for designing improved materials properties.

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