

Superglide at an internal incommensurate boundary

Frédéric LANÇON¹, Jia YE^{2,3}, Damien CALISTE¹, Tamara RADETIC²,
Andrew M. MINOR^{2,3}, Ulrich DAHMEN²

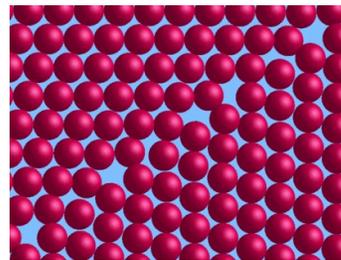
¹*Laboratoire de simulation atomistique (L_Sim), SP2M, INAC, CEA, 38054 Grenoble, France.*

²*National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, Ca 94720, USA.*

³*Department of Materials Science and Engineering, University of California, Berkeley, Ca 94720, USA*

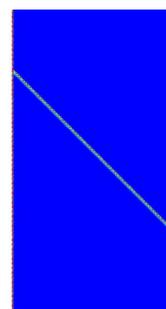
This document contains one additional figure (S1) and the legends of the five movies (M1-M5) available as supplemental material of our article. Each movie legend consists of the movie file name and a descriptive caption. It is illustrated in this document by a still image.

Movie 1 (M1-hypofriction-movie): Atomic displacements at a $\sqrt{2}$ type incommensurate grain boundary in gold during grain sliding in hypofriction condition. They can be view as trajectories at zero temperature since the grain boundary

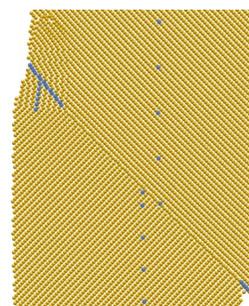


stays in its ground state. Atomic trajectories have been obtained by a minimum energy path technique [Ulitsky A. and Elber R., *J. Chem. Phys.*, **92** (1990) 1510]. The movie corresponds to figure 1.

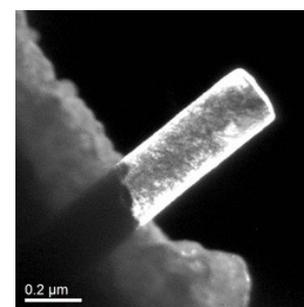
Movie 2 (M2-nanopillar_model-movie): Grain sliding during simulation of a gold pillar compression. Local atomic energy is indicating by color (all atoms with energy above the cohesion energy by more than 2% have a color that saturates to red). The length of the grain boundary in this 239/169 model is 69 nm. The movie corresponds to figure 2.



Movie 3 (M3-nanopillar_model-zoom-movie): Grain sliding during simulation of a gold pillar compression. Only one atomic plane in depth is represented and some atoms are specially marked to emphasis their respective displacement. The length of the grain boundary in this 99/70 model is 28 nm. The movie corresponds to figure 2.



Movie 4 (M4-nanopillar_monocrystal): Single crystal pillar deformation during compression in the transmission electron microscope. The diameter of the gold pillar is approximately 200 nm. The movie corresponds to figure 4.



Movie 5 (M5-nanopillar_polycrystal): Grain boundary sliding during compression of a polycrystal pillar in the transmission electron microscope (dark field condition). The diameter of the gold pillar is approximately 200 nm. The movie corresponds to figure 4.

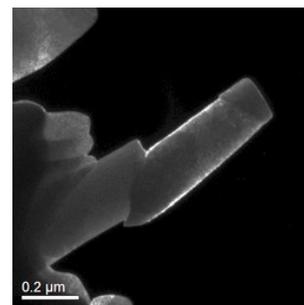
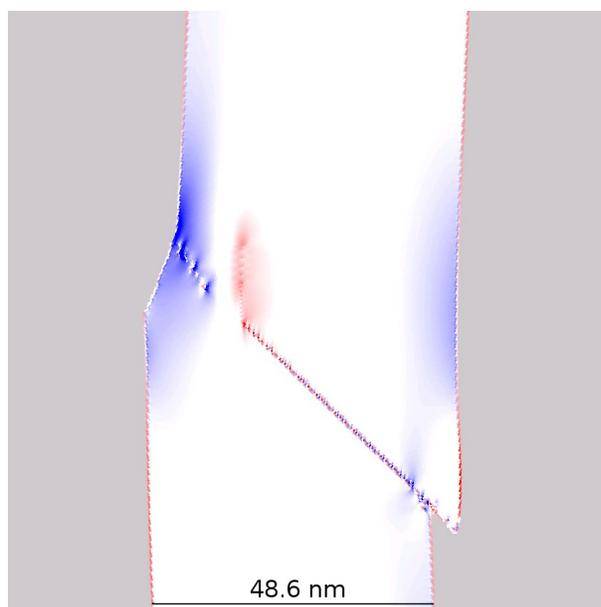


Figure S1: Compressive stress field σ_{zz} during a gold pillar compression (239/169 model) showing how the stress is connected to the reconstruction zones at the edges of the $\sqrt{2}$ grain boundary. Local stress is indicating by colour (blue and red indicate compressive and tensile stresses respectively). The local stress, σ_{zz}^i at atom i , is defined from the virial expression as $\sum_j F_z^{ij} z^{ij} / (2 v_0)$, where F^j is the contribution



due to atom j to the force acting on i (and F_z^{ij} is its z -component), z^{ij} is the vertical component of the vector r^{ij} , and v_0 is the atomic volume at zero stress. The average stress $\langle \sigma_{zz}^i \rangle$ is equal to -0.80 GPa (compressive). On the figure, the blue and red colours saturate at ± 8 GPa.

Acknowledgements All model representations have been obtained with the free visualization software V_Sim (http://inac.cea.fr/L_Sim/V_Sim/index.en.html in 2009).