

Structure of finite-size $\Sigma 3$ grain boundaries and their interactions with dislocations

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Because material structure determines material properties, it is important to investigate the effect of size on the structure of crystalline defects. Nanocrystalline materials have indeed raised the issue of finite size effects on the behavior of grain boundaries and dislocations during deformation. Nanocrystalline materials deform by grain boundary accommodation possibly accompanied by dislocation slip originating from grain boundaries. However the exact role of dislocation activity has not yet been clarified. The complexity comes from the small length scale involved during deformation of nanocrystalline materials, where the effects of neighboring defects on grain boundary dislocation interactions need to be taken into account.

Specifically, previous transmission electron microscopy works have demonstrated that the $\Sigma 3$ $\{112\}$ grain boundary can relax through a lattice translation [1]. However, these studies, based on isolated observations of $\Sigma 3$ $\{112\}$ boundaries, have painted a conflicting picture with reported translations ranging from zero to half the $\{111\}$ plane spacing [2]. Using high-resolution transmission electron microscopy (HREM), we measured local translations along $\{112\}$ boundaries of varying sizes in Au thin films (Fig. 1a). The structural profile of the boundary is explained using continuum elasticity theory and first-principles calculations as originating from a competition between elastic energy and the energy cost of forming continuous planes across the boundary [3]. This competition leads to a structural transition at a critical grain boundary size, in agreement with the experiments (Fig. 1b). We have shown that finite size effects play a strong role in grain boundary physics, leading to a structural transition as a function of grain boundary size. This work points out the role of elastic strains in controlling the behavior of small boundaries, which will affect the interaction between dislocations and grain boundaries during deformation of nanocrystalline materials.

Indeed, using HREM observations and embedded atom method (EAM) simulations, study of the $1/3\langle 111 \rangle$ dislocation equilibrium structure near $\{112\}/\{111\}$ grain boundary junctions in Au thin films provides experimental evidence that local environment affects the dislocation structural relaxation and its interactions with neighboring grain boundaries. The $1/3\langle 111 \rangle$ dislocation is assimilated into the $\{112\}$ grain boundary unless a second $\{111\}/\{112\}$ junction is present, in which case, the $1/3\langle 111 \rangle$ dislocation dissociates by emitting a Shockley partial dislocation reacting with the second junction followed by an extended stacking fault (Fig. 2). The stability of this defect is explained by relaxation of the elastic strains at the boundary junctions due to the $\{111\}$ plane offset that exists at the stacking fault. The predicted maximum distance between interacting junctions is consistent with the experimental observations. This extended defect is the first step of a twinning mechanism and constitutes a pinning mechanism as well for the twin boundaries. It is also the first experimental evidence of long-range interactions between adjacent grain boundaries through dislocation emission, which has been previously predicted by molecular dynamic simulations [4].

- [1] A. P. Sutton and R. W. Balluffi, Interfaces in Crystalline Materials (Oxford University Press, 1996).
- [2] H. Ichinose and Y. Ishida, Phil. Mag. A 52 (1985) 51
- [3] E.A. Marquis, J. C. Hamilton D.L. Medlin, F. Léonard, PRL 93, 15 (2004) 156101
- [4] Van Swygenhoven H., Science 296 (2002) 66
- [5] Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

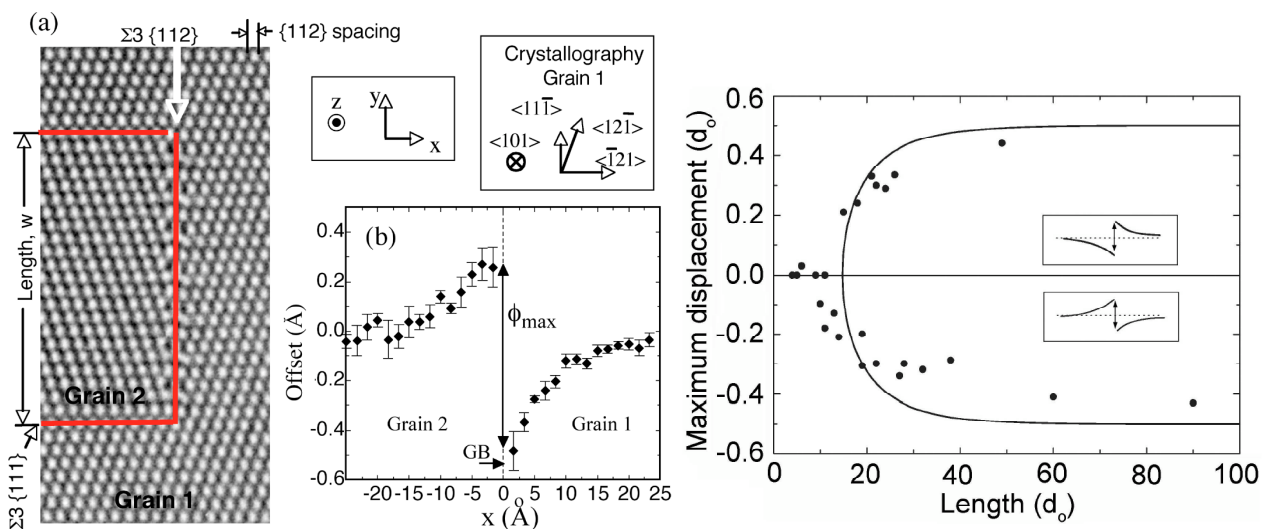


Fig.1 (a) HREM observations of a Au $\{112\} \Sigma 3$ twin boundary bounded by two $\{111\} \Sigma 3$ twin boundaries. (b) Average of the y-component of the displacement along 6 $\{111\}$ planes in the middle of the boundary as a function of distance from the $\{112\}$ boundary. (c) Maximum displacement along the $\{112\}$ boundary plane as a function of the boundary length showing the structural transition for lengths $\sim 20d_0$ (where d_0 is the $\{111\}$ plane spacing)

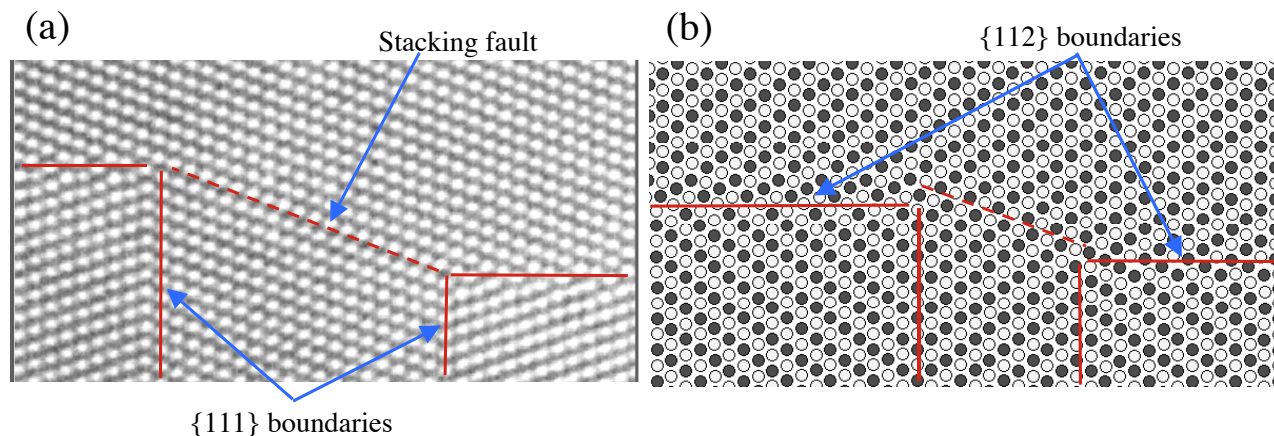


Fig. 2 (a) HREM observations and (b) EAM simulation of an extended stacking fault between two $\{111\}/\{112\}$ junctions in Au.