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DOI: 10.1017/S1431927606068929

Microsc Microanal 12(Supp 2), 2006

Strain relief at finite-sized grain boundaries drives dislocation emission

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Whether dislocation- or grain boundary- mediated plasticity operates during deformation of nanocrystalline materials is still a matter of debate [1]. The complexity arises from the small length scales involved during deformation of nanocrystalline materials, where the effects of neighboring grain boundaries on dislocation behavior need to be taken into account. Extended stacking faults forming between grain boundaries are one example of such interactions. Here, we focus on the particular case of stacking faults forming between {111} and {112} twin boundaries junctions in Au thin films.

A representative example of the extended stacking fault joining two junctions between {111} and {112} twin boundaries is shown in FIG 1. A burgers' circuit around the entire structure yields a closure failure equal to 1/3<111>, and an extra {111} plane can be observed on the left side of the extended stacking fault. The length of these stacking faults varies from 0.5 to 8 nm, which is a surprisingly large value compared to the length of a Au stacking fault separating to partial dislocation resulting from the dissociation of an edge dislocation (e.g. 1.8 nm).

The presence of the $1/3<111>$ twin boundary dislocation is not surprising as it can be formed from the impingement of a lattice dislocation on a {111} twin boundary [1]. The {112] boundary has a relaxed structure exhibiting an offset of the {111} planes equal to ½ {111} plane spacing [2]. If a 1/3<111> dislocation is located at a {111}/{112} boundary junction, it is incorporated into the {112} boundary. The energy component due to the GB γ-surface is not modified since the profile of the {111} plane offset in the case of a dislocation-containing boundary is comparable to the profile of a defect-free boundary (FIG. 2); the difference being the sign of the offset at one of the junctions. In the case of the defect-free boundary, the profile can be modeled by a dislocation dipole +/- 1/6<111> while for the dislocation- containing boundary, the offset profile can be compared to that created by two 1/6<111> dislocations of the same sign. The incorporation of the 1/3<111> dislocation leads to a decrease in strain energy proportional to $b_{1/3<111>}^2$.

If a second {112} boundary is present, a 1/3<111> dislocation positioned at the {111}/{112} junction emits a Shockley partial dislocation that extends to the {111}/{112} junction of the second twinned grain. The {111} plane offset that exists at the two {112} boundaries is then continuous through the stacking fault that has itself created an offset equal to 1/3 {111} plane spacing. The stability of this long stacking fault is explained by the decrease of elastic strains that exists at the {111}/{112} junctions. The energy decrease due to strain relaxation is compensated by the energy increase due to the creation of the staking fault leads to a condition on the maximum length of the stacking fault. This is the first experimental evidence of long-range interactions between adjacent grain boundaries through dislocation emission, which has consequences not only on grain boundary interactions in nanocrystalline materials, but also on grain boundary mobility.

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[4] Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed-Martin Company, for the United States Department of Energy National Nuclear Security Administration under contract DE-AC04-94AL85000.

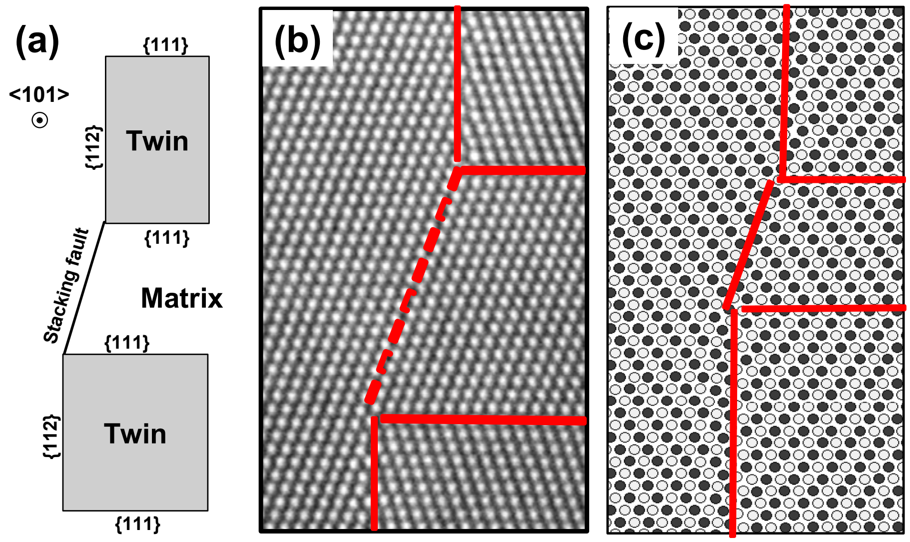

FIG. 1. Extended stacking fault between two {111}/{112} boundary junctions. (a) schematic of the defect; (b) HREM image ; (c) EAM simulation.

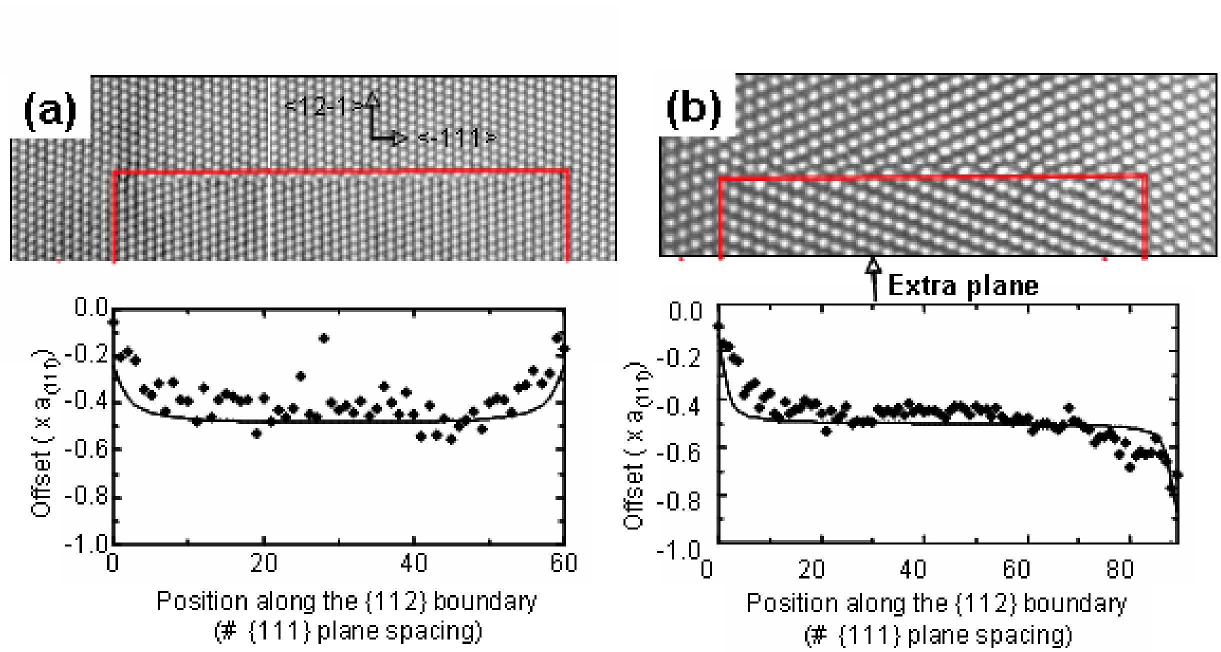

FIG. 2. HREM images and {111} plane offset profiles for (1) defect free {112} grain boundary and (b) {112} boundary containing a 1/3<111> dislocation. The lines corresponds to the expected displacement from a Pieirls-Nabarro model for (a) a 1/6<111> dislocation dipole and (b) two 1/6<111> dislocations of same sign,

https://doi.org/10.1017/S1431927606068929 Published online by Cambridge University Press