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Analysis of Stresses and Strains around Dislocations at Grain Boundaries by Quantitative High-Resolution Electron Microscopy

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In order to analysis stresses and strains across grain boundaries, the geometric phase technique has been adapted with respect to the case of an isolated dislocation [1]. A high-resolution image of a dislocation constricted at a coherent twin boundary in germanium can be seen in Fig. 1. Due to the grain boundary, a unique reference lattice cannot be defined for the whole field of view. Geometric phase images were therefore calculated first in grain I using the lattice shown, taken far from the boundary, and the strain field calculated. A reference lattice for grain II was determined by applying the perfect orientation relation for a twin boundary to the reference used in grain I, similar to the procedure used in circuit mapping [2]. Strains were then calculated in grain II. Finally, strain fields from grain I and II were assembled piece-wise to produce the overall strain maps (see Fig. 1). Note that the reference is identical for the x-axis parallel to the common {111} lattice fringes.

The measured strains were compared with isotropic elastic calculations for an isolated matrix dislocation of the same Burgers vector (Fig. 1). Whilst strains in the grains on either side of the twin boundary agree closely with the isolated dislocation case (to within 0.2% at 2.5 nm spatial resolution), significant additional strains are localised at the boundary plane for the perpendicular component ε_{xx}: the boundary expands and contracts more than the surrounding matrix. We can discount image artifacts for this component as the lattice fringes used for the analysis are common to both crystals and hence are affected in an identical fashion by the lens. In addition, it is difficult to imagine why artifacts would reverse from expansion to contraction above and below the dislocation.

Stresses were determined using linear anisotropic elastic theory, and bulk elastic constants, from the strains measured in grains I and II. The boundary is in mechanical equilibrium so certain relations must apply across the boundary plane [3]. The dislocation, in effect, applies large compressive and tensile stresses to the boundary (Fig. 2a). By comparing the matrix stresses and boundary strains (Figs. 2b and 2c), values for the effective elastic modulus of the twin boundary are proposed. It is found that the boundary is significantly weaker than the matrix, and can be interpreted in terms of the non-equilibrium configuration of the boundary. An extension of the method is proposed to measure more generally the elastic properties of grain boundaries and interfaces.

References

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[4] GPA phase plug-in for DigitalMicrograph (Gatan) available from HREM Research: www.hremresearch.com

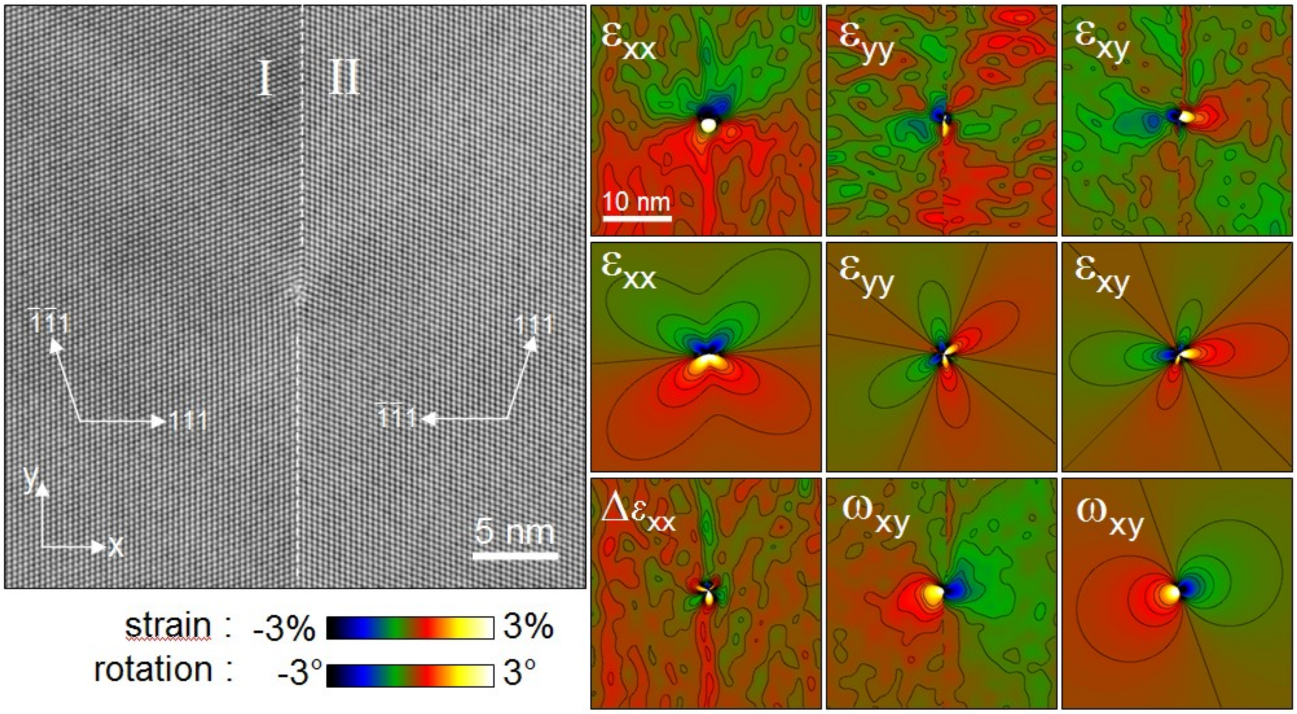

FIG. 1. Strain analysis of a dislocation located at a coherent Σ3 twin boundary in germanium: HREM image taken on a JEOL 200CX, reference lattice for grains I and II indicated; local strain and lattice rotation maps, experimental (noisy) and from isotropic elastic theory, contours every 0.2% strain and 0.2° rotation. Difference $\Delta\varepsilon_{xx}$ between ε_{xx} experiment and theory also shown.

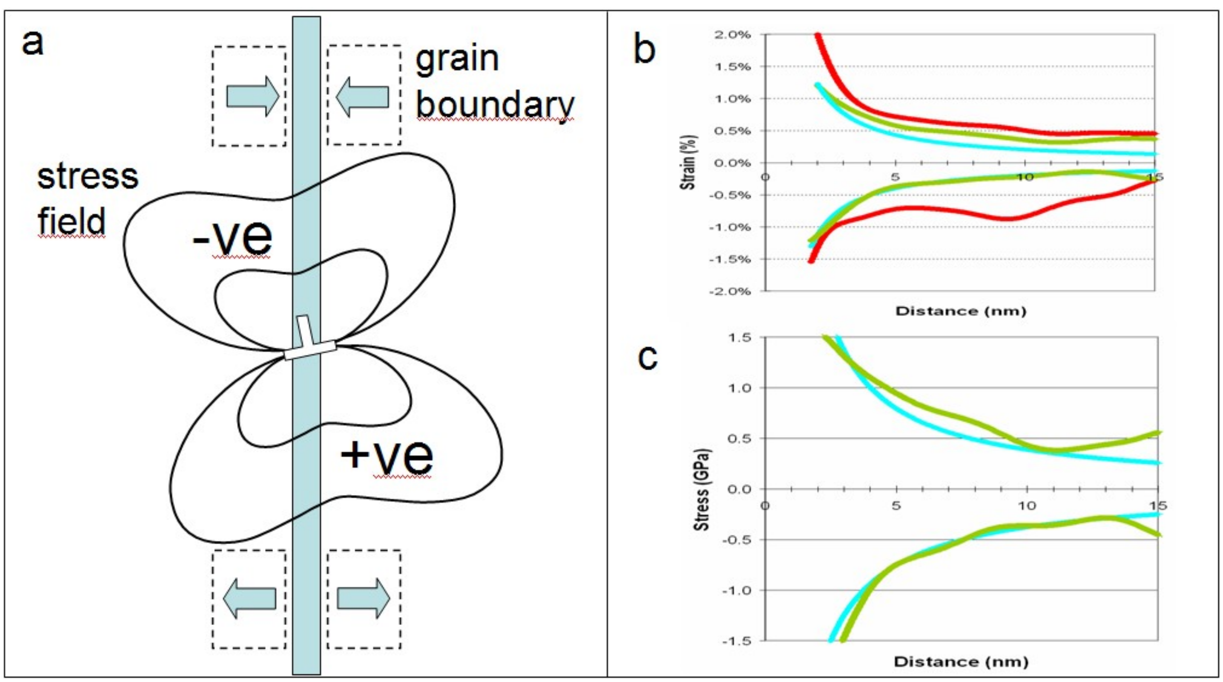

FIG. 2. Grain boundary stress analysis: (a) diagram showing compressive and tensile stresses applied to the boundary due to the dislocation; (b) strains measured along boundary: at boundary plane (red), in adjacent matrix (green), theoretical (blue); (c) stresses applied to boundary: measured (green), theoretical (blue). Strains are significantly higher at boundary than in surrounding matrix.

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