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Local Strain and Rotation at Low-Angle Grain Boundaries

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Low-angle grain boundaries (LAGBs) profoundly affect the mechanical, chemical, and electrical properties of their host materials. The properties of LAGBs are understood in terms of their constituent dislocations, which accommodate small misorientations between grains. Discrete dislocations result in a heterogeneous local structure along the boundary. We examined the structure of a LAGB in the mineral olivine [$(Mg,Fe)_2SiO_4$] using geometric phase analysis (GPA), an image-processing technique for mapping displacement and strain from high-resolution transmission electron microscopy (HTREM) images with high accuracy and nanometer spatial resolution.

GPA has been used to measure displacement fields around edge dislocations in Si to 3 pm [1] and in olivine to 9 pm [2] accuracy. Given the displacement field, the local planar strains and rigid-body rotation are determined by numerical differentiation of displacements [3]. Careful calibration of the microscope's lens distortions allows quantification of strains to < 1% and rotation to 0.3° across the entire field of view [4].

The LAGB in our olivine sample lies close to the $(10\bar{1})$ plane and consists of alternating **a** and **c** edge dislocations (Fig. 1a). The rotation map (Fig. 1b) gives the local orientation of the crystal with respect to the median lattice. The contours reveal the complex corrugation of the boundary as it snakes from dislocation to dislocation. The medium-range dilatational (ε_{xx}, ε_{yy}; Fig. 1c,e) and shear strains (ε_{xy}; Fig. 1d) show the extension of each strain component into the surrounding material and the interactions of the dislocations along the boundary.

The analysis revealed a boundary that is corrugated rather than planar. Elastic calculations show that this waviness is independent of the host material. Based on our observations and analysis, we provide equations for the boundary position, local curvature, and the lattice rotation field for any LAGB [5]. The rotation and strain mapping results provide the basis for a re-examination of grain-boundary properties in materials such as high-temperature superconductors, metals, and naturally deformed minerals at the nanoscale.

References

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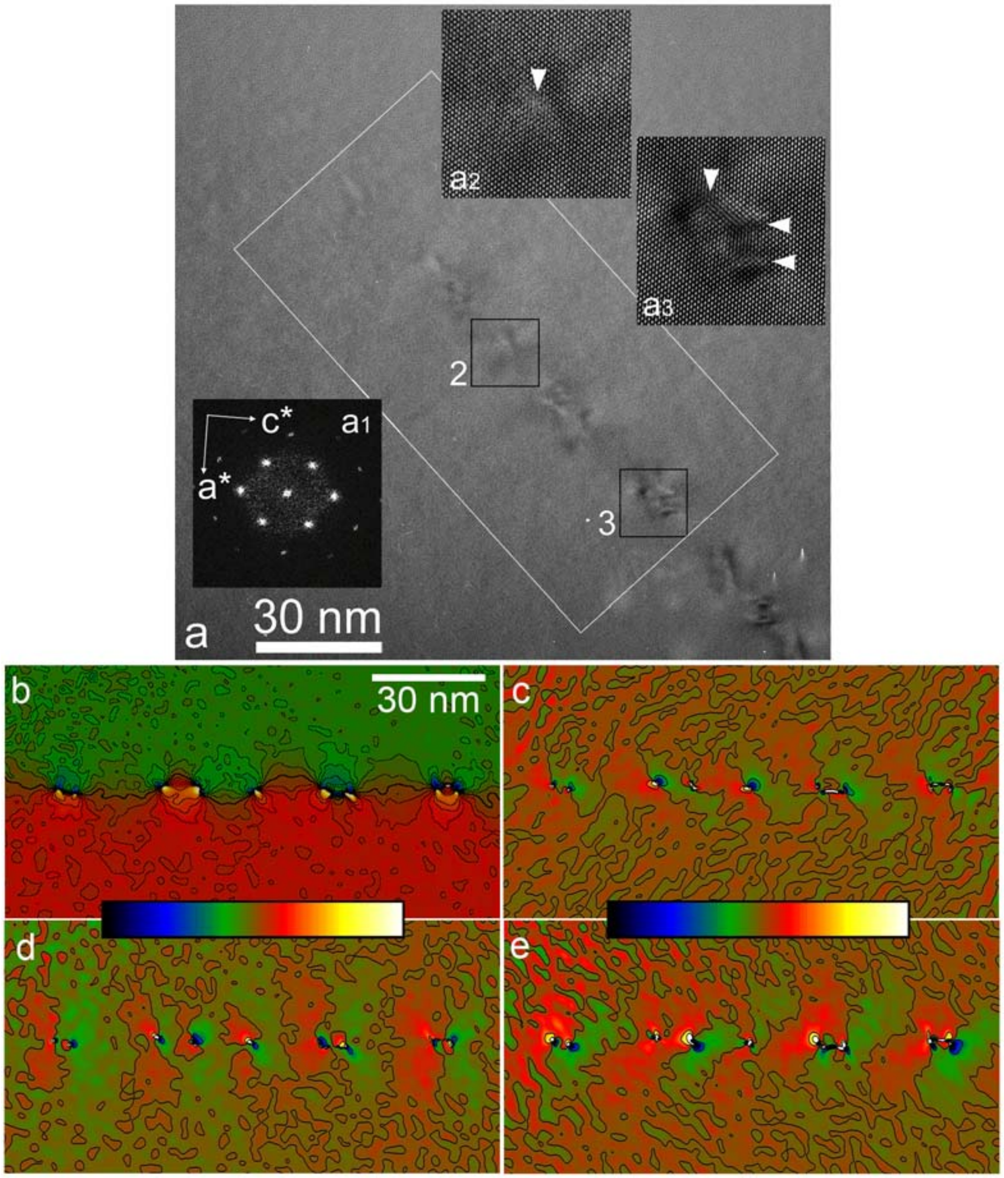

FIG. 2. (a) HRTEM image of olivine shows faint strain contrast around dislocations that are oriented parallel to the viewing direction. The dislocations comprise a LAGB that accommodates a 1.5º rotation between the two adjacent crystals. (inset) The digital diffractogram of the image indicates the average orientation of the sample. (a1) The magnified view of the region marked ‘1’ in (a) shows a [100] dislocation (arrowed). (a2) The magnified view of the region marked ‘2’ in (a) shows closely spaced [100] and [00-1] dislocations (arrowed). The [00-1] dislocation is weakly dissociated (horizontal arrows). The rotation map (b) gives the local orientation of the crystal. The waviness of the boundary is evident from the 0º contour (bold), which is the trace of the boundary. Contours are every ±0.3º on either side of the 0º contour to ±0.6º; the color bar indicates the full range of ±12º. The strain maps (ε_{xx}, ε_{xy}, and ε_{yy}; c, d, and e, respectively) show the medium-range strain around the dislocations. Contours are every ±2% on either side of the 0% contour to ±0.4%; the color bar indicates the full range of ±5%.

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