Characterization of lattice rotations and distortions from a single dislocation

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Abstract

Understanding and controlling the behavior of dislocations is crucial for a wide range of applications. Quantitative X-ray diffraction measurements of the strain fields due to individual dislocations, particularly in the bulk, however, have thus far remained elusive. Here we report the first characterization of a single dislocation in a freestanding GaAs/$In_{0.2}Ga_{0.8}As$/GaAs membrane by synchrotron X-ray micro-beam Laue diffraction. Our experimental X-ray data agrees closely with textbook anisotropic elasticity solutions for dislocations, providing one of few experimental validations of this fundamental theory. On the basis of the experimental uncertainty in our measurements, we predict the X-ray beam size required for three-dimensional measurements of lattice strains and rotations due to individual dislocations in the material bulk. These findings have important implications for the *in-situ* study of dislocation structure formation, self-organization and evolution in the bulk.

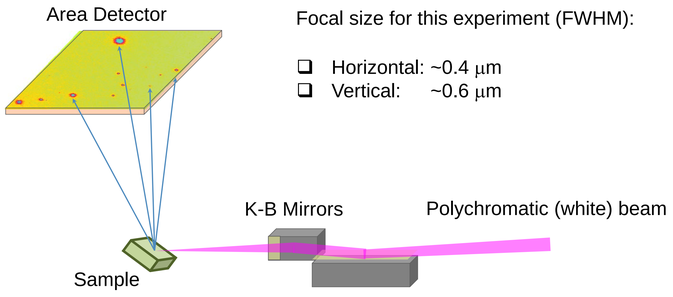
Dislocations

Dislocations are crystallographic defects that allow the minimization of strain energy through the localization of crystal lattice distortion. Their behavior is of fundamental importance for the performance of thermoelectric devices, nano-electronics and solar cells. In structural engineering alloys, used for high-performance aerospace applications, dislocation-mediated slip is one of the main deformation mechanisms. Careful management of dislocation structures and their evolution is essential to optimizing material strength and resistance to failure.

Transmission Electron Microscopy (TEM) revolutionized Materials Science by allowing the visualization of individual dislocations in thin, electron transparent samples. However small sample size may lead to size effects that modify dislocation behavior. The greater penetration depth of X-rays potentially allows the study of dislocations in samples more representative of the material bulk. However, thus far quantitative X-ray measurements of the strain fields surrounding individual dislocations have remained elusive.

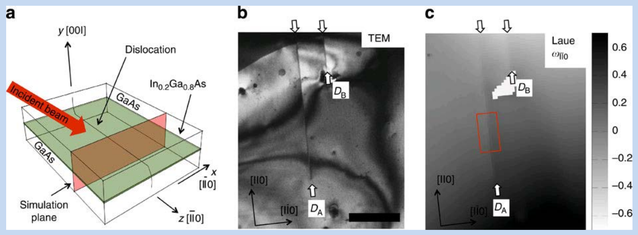
X-ray Micro-beam Laue Diffraction

Synchrotron X-ray micro-beam Laue diffraction (XMD) is perfectly suited to the mapping of polycrystalline samples and the study of steep orientation gradients. It uses a focused, polychromatic X-ray beam to probe submicron-sized scattering volumes. By fitting of the diffraction peak positions on an area detector, it allows the determination of all three lattice rotation components and the full deviatoric strain tensor at each data point with a single exposure.



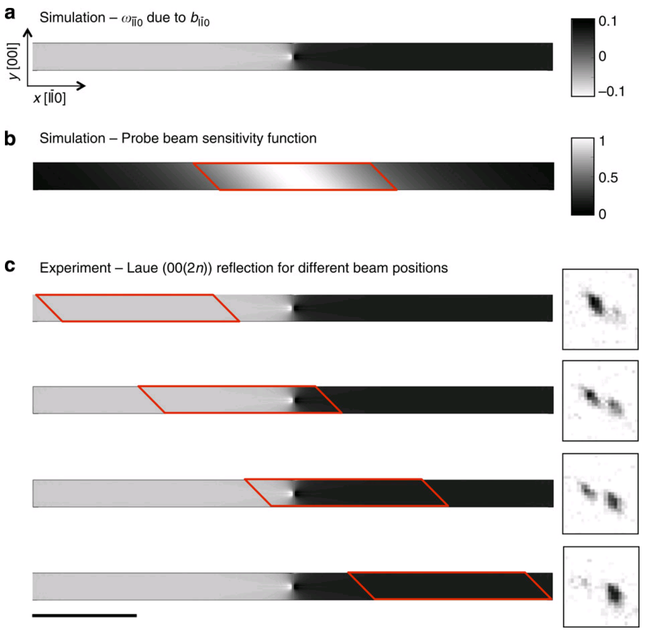
Focal size for this experiment (FWHM):

- Horizontal: ~0.4 μm
- Vertical: ~0.6 μm

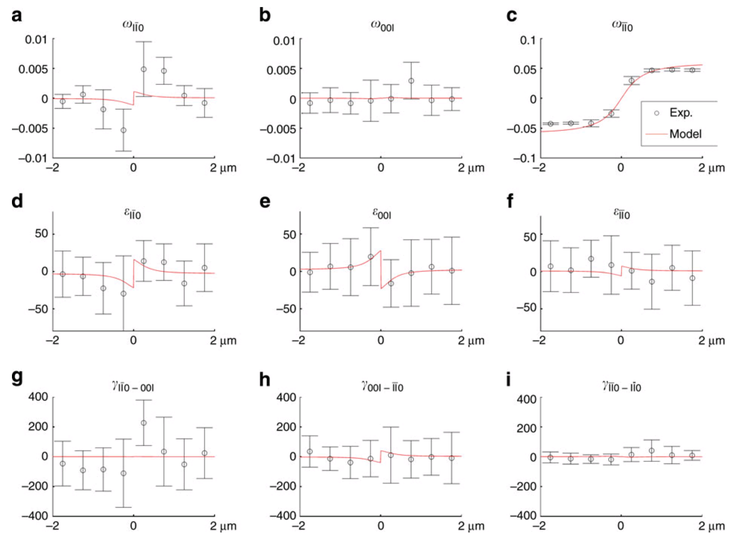


A freestanding membrane of GaAs/$In_{0.2}Ga_{0.8}As$/GaAs, 60 nm/9.5nm /60 nm.

- Lattice mismatch between GaAs and $In_{0.2}Ga_{0.8}As$ layers gives rise to misfit dislocations at their interface (schematically shown in Fig.a).
- Two of such dislocations clearly identifiable in the TEM image (Fig. b).
- Map of lattice rotation measured by x-ray microdiffraction over the same area show clear contrast across the dislocations (Fig. c). Further strain measurements were carried out inside the red rectangle.



a. Simulated lattice rotation across the dislocation;
b. Simulated beam sensitivity function. Red parallelogram showing the FWHM;
c. Experiment images of the (00(2n)) reflection recorded as the x-ray probe moved across the dislocation line.

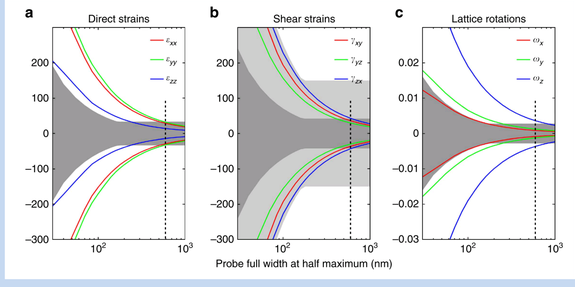


(a-c) *Lattice rotations (in degrees) about crystal axes [I$\bar{1}$0], [00I] and [$\bar{1}\bar{1}$0], repsectively;*
(d-f) *Direct elastic strains (in units of 10^{-6}) along [I$\bar{1}$0], [00I] and [$\bar{1}\bar{1}$0] directions, respectively;*
(g-i) *Shear strains in the ($\bar{1}\bar{1}$0), (I$\bar{1}$0) and ($\bar{1}\bar{1}$0) planes, respectively;*
Red lines are theoretical simulations with an anisotropic elastic model; dots with error bars are measured by experiment. Error bars are obtained by comparing 16 different line scans across the dislocation line (within the rectangular area marked on the sample image above).

- With micro-beam x-ray Laue diffraction, this experiment demonstrates the first imaging of the rotation and strain field surrounding a single dislocation.
- The measured rotation and strain field provide validation of the theoretical models.
- A demonstration of the current capability/sensitivity of the microdiffraction technique.
- With a depth-resolving differential aperture, the same measurement is feasible with 3D resolution in bulk materials in the future.

The ability to measure single dislocation strain fields in the bulk in 3D would open up revolutionary possibilities for the *in-situ* study of dislocation behavior, structure formation and self-organization.

Smaller focal size is the key to the future



(a-c) *Estimated minimum and maximum strain and lattice rotation values for a misfit dislocation buried in the bulk, as functions of the size of the x-ray probe. Grey areas represent estimated uncertainties.*

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