Comment on "Bulk Dislocation Core Dissociation Probed by Coherent X Rays in Silicon"

In a recent Letter [1], Jacques and co-workers report on the investigation of dislocation core dissociation in silicon using coherent x-ray diffraction. In this study, a dislocation is found to be dissociated in two partials distant by "several hundred nanometers." This finding is puzzling and requires some comments, as it is very far from the usually acknowledged value of few nanometers. The authors present this measure as characteristic of "bulk dislocations," in contrast to the "surface dislocations" that are supposedly probed by electron beams.

The mechanism of dislocation dissociation is explained by the elastic theory of dislocations [2]. In a stress-free crystal at equilibrium, the core of a perfect dislocation splits in two partial dislocations to minimize the elastic energy of the crystal. The dissociation width is determined by a balance between the repulsive interaction between partials and the attractive force that tends to reduce the width of the intrinsic stacking fault ribbon connecting the two partials. As a consequence, the dissociation width is inversely proportional to the stacking fault energy. Available measurements performed by transmission electron microscopy, in weak-beam conditions or in high-resolution transmission mode, indicate that the dissociation widths in silicon range from 4 to 8 nm depending upon the orientation of the perfect and partial dislocations [3,4]. Elastic theory then yields a stacking fault energy of about $50\ \mathrm{mJ\,m^{-2}}$, in good agreement with values of $75\ \mathrm{mJ\,m^{-2}}$ [5] and $38\ \mathrm{mJ\,m^{-2}}$ [6] predicted by first-principles computations.

Jacques *et al.* justify the discrepancy between their measurement and previous ones by suggesting that electron microscopy methods are limited to surface investigations, in contrast to x-ray methods. However, in the vast majority of electron microscopy observations, the dislocations are truly bulk defects that are present in the material before thin foil preparation. As this last process is typically performed at 300 K, dislocations are immobile and no change in dissociation width is expected. One could argue about possible local stress changes in bent samples affecting weak-beam conditions, but this effect is negligible in the high-resolution transmission mode where the observed dislocation lines are perpendicular to the specimen surfaces.

Besides, assuming the dissociation width to be "several hundred nanometers," the stacking fault energy should accordingly be 2 orders of magnitude lower than currently accepted values. This would, however, imply that electronic structure calculations like density-functional theory fail to simulate stacking faults in silicon. This would be in contradiction with numerous studies that demonstrated the accuracy of such methods to estimate defect-related properties in many materials, including silicon.

The observation of a large dissociation width by coherent x-ray measurement reported in [1] is more likely to be explained by assuming that the investigated dislocation is not at equilibrium in a pure, stress-free, bulk silicon sample. The observed distance between partial dislocations would then result from the specific treatment that introduced dislocations in the sample—that is, high temperature annealing in an oxygen atmosphere. In that case, partial dislocations are separated by an extrinsic stacking fault induced by oxidation processes [7]. In such conditions, the dissociation widths are governed by diffusion processes and dislocation climb. Alternatively, dissociation widths of several hundreds of nm can be reached by a pure glide process in very specific conditions, like large applied stresses on pinned dislocations [8,9], conditions which are not relevant to the present investigation.

For all these reasons, it does not seem justified to generalize the observation made in [1] to dislocations in silicon, as well as to suggest without a cross-check on the same sample that electron microscopy only allows "surface dislocation" examinations. However, we wish to point out that the present comments do not question the potentiality of coherent x-ray methods for investigating the fine structure of dislocations.

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