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The effect of residual lens aberrations on the determination of column positions around partial dislocations in GaAs

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In recent years, it became possible to extend the resolution of field emission microscopes into the sub Ångstrom region by reconstruction of the electron exit wave from a focus series of lattice images [1-4]. This improved resolution makes it desirable to revisit imaging and analyses of dislocation core structures with truly atomic resolution. A clarification of the atom arrangements in dislocation cores is a long standing problem [5].

A focus series of lattice images from edge-on dislocations in GaAs:Be were recorded using the Philips CM300 FEG/UT microscope at National Center for Electron Microscopy. Figure 1 is a phase image of a reconstructed electron exit wave from a wedge shaped GaAs sample that shows two partial dislocations with the adjacent stacking fault. Both partial dislocations are of 30° character as determined by a Burgers circuit. The inserted extra half plane ends between narrowly spaced (111) planes revealing a glide-set configuration. Figure 2 shows a second example with a stacking fault intersecting the sample surface and a 30° Ga terminated partial dislocation. We explore a quantitative characterization of 30^0 partial dislocations by matching experiments with *ab initio* electronic structure total energy calculations employing ultrasoft pseudo potentials [6, 7]. Combining the *ab initio* results with simulation software enables calculations with a similar number of atoms as recorded in the experiment [8]. Agreement between theory and experiment is quantified by comparing column positions extracted from experiment and simulation. It is of special interest to estimate the effect of residual lens aberrations on our ability to match column positions. Hardware corrections of lens aberrations by an analyses of Thon rings allow for control of residual distortions in the reconstructed exit wave image to about 50 pm. Such measurements become unreliable if the residual distortions are smaller. In this case, a comparison with theory is utilized that reveals discrepancies of ~ 20 pm between calculated and measured column positions at non-periodic lattice sites indicating that the residual distortions are around such lower values. A further reduction of image distortions by aberration correction through software is as shown in Figure 3 and will be discussed [9, 10].

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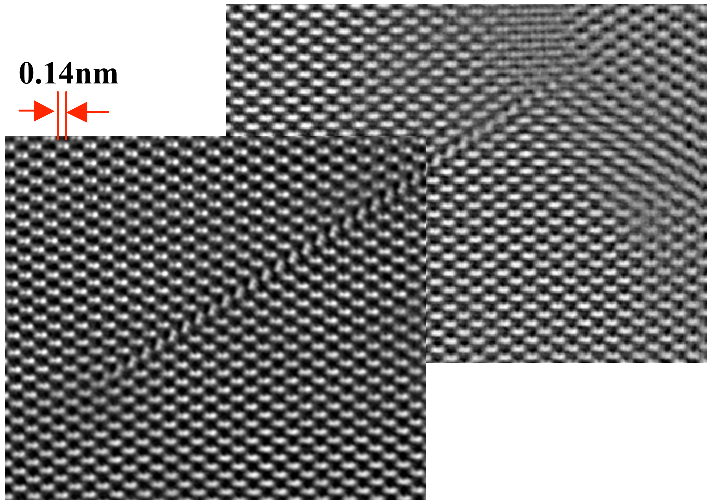

FIG. 1. Phase image of the reconstructed electron exit wave with two 30° partial dislocations at the ends of a stacking fault in GaAs: Be (Projection orientation [011]).

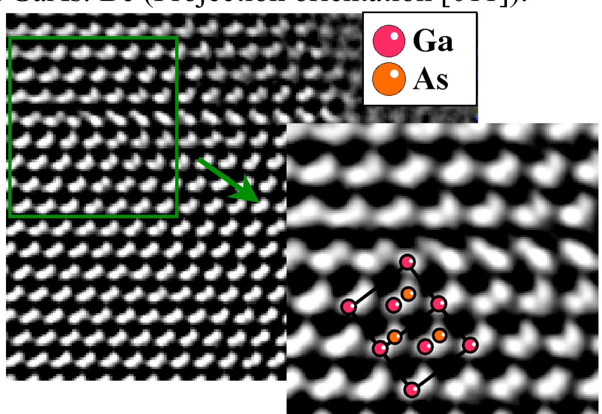

FIG. 2. Phase image of the reconstructed electron exit wave with stacking faults and partial dislocation in GaAs: Be (Projection orientation [011]). The inset shows enlarged image of the partial dislocation at the end of an intrinsic stacking fault.

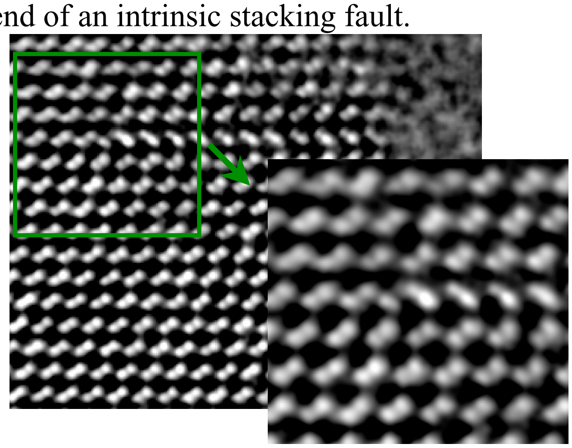

FIG. 3. Phase image of the reconstructed electron exit wave with stacking faults and partial dislocation in GaAs: Be (Projection orientation [011]) by aberration correction with software.