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Atomic-Resolution Imaging in the Aberration-Corrected BNL JEM2200FS

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Our ability to study complex structures in a scanning transmission electron microscope (STEM) is not only limited by the smallest possible probe-size that can be formed in the objective lens system, but also by the specimen and scanning-system instabilities, as well as environmental factors such as thermal stability and electro-magnetic fields. When the BNL-JEM2200FS, equipped with a CEOS STEM-corrector [1] was installed in 2005, particular attention was paid to minimize the instrument's electronic instabilities, reduce the ambient electro-magnetic field, and decrease the airflow across the column. [2]

Figure 1 shows two Z-contrast images of Si (110) taken before and after modifying the room-environment, as well as the microscope's scanning system. The Si-dumbbells in Fig. 1a are not resolved and large sinusoidal distortions of the atomic columns are visible. Figure 1b shows a similar view of Si (110), but now the atomic columns are clearly separated and the image distortions are mostly eliminated. A FFT of Fig. 1b is shown in Fig. 1c, where the (200), the (400) as well as the (511) spots are clearly visible, indicating a probe-size of 1.05 Å. The remaining objective lens aberrations after the corrector tuning are: C_1 (defocus) = -1.054 nm, A_1 (2-fold astigmatism) = 23.68 nm, A_2 (3-fold astigmatism) = 60.43 nm, B_2 (axial coma) = 15.04 nm, C_3 (spherical aberration) = -134.7 nm, A_3 (4-fold astigmatism) = 950.3 nm, S_3 (star aberrations) = 614.4 nm, and A_4 (5-fold astigmatism) = 28.3 µm. The corresponding calculated phase-plate with these parameters is shown in Fig. 1d. Here the inner ring indicates a 20 mrad diameter, while the outer ring indicates 63mrad. For high-resolution Z-contrast imaging, a probe convergence angle of 15mrad and a detector inner angle of collection angle of ~100mrad are chosen.

One application of atomic-resolution Z-contrast imaging is shown in Fig. 2. Here, five monolayers of $SrTiO_3$ (001) can be seen on As-terminated GaAs (110). Such a structure is of particular interest to the semiconductor industry due to its potential application as a novel high-κ dielectric/ semiconductor interface that could provide a thermodynamically and electrically stable alternative to current silica-based technologies. Fig. 2a shows that the hetero-interface is atomically flat and no significant diffusion between the film and the substrate is visible. The image does not show any obvious surface reconstruction of the support (Fig 2 c and d show models of the energetically favorable reconstructions in As-terminated GaAs, β and β2), but rather a flat interface with $SrTiO_3$ film. A simple model of the interfacial atomic structure based on the Z-contrast is shown in Figure 2b. While the $SrTiO_3$ film appeas to be highly oxygen deficient, Fermi-level remains unpinned at the interface after a Ti-prelayer deposition.[3] The potential effect of O-vacancies on the As-dimer formation and the interfacial density of states will be shown by atomic-column resolved EELS in combination with density-functional theory calculations. [4]

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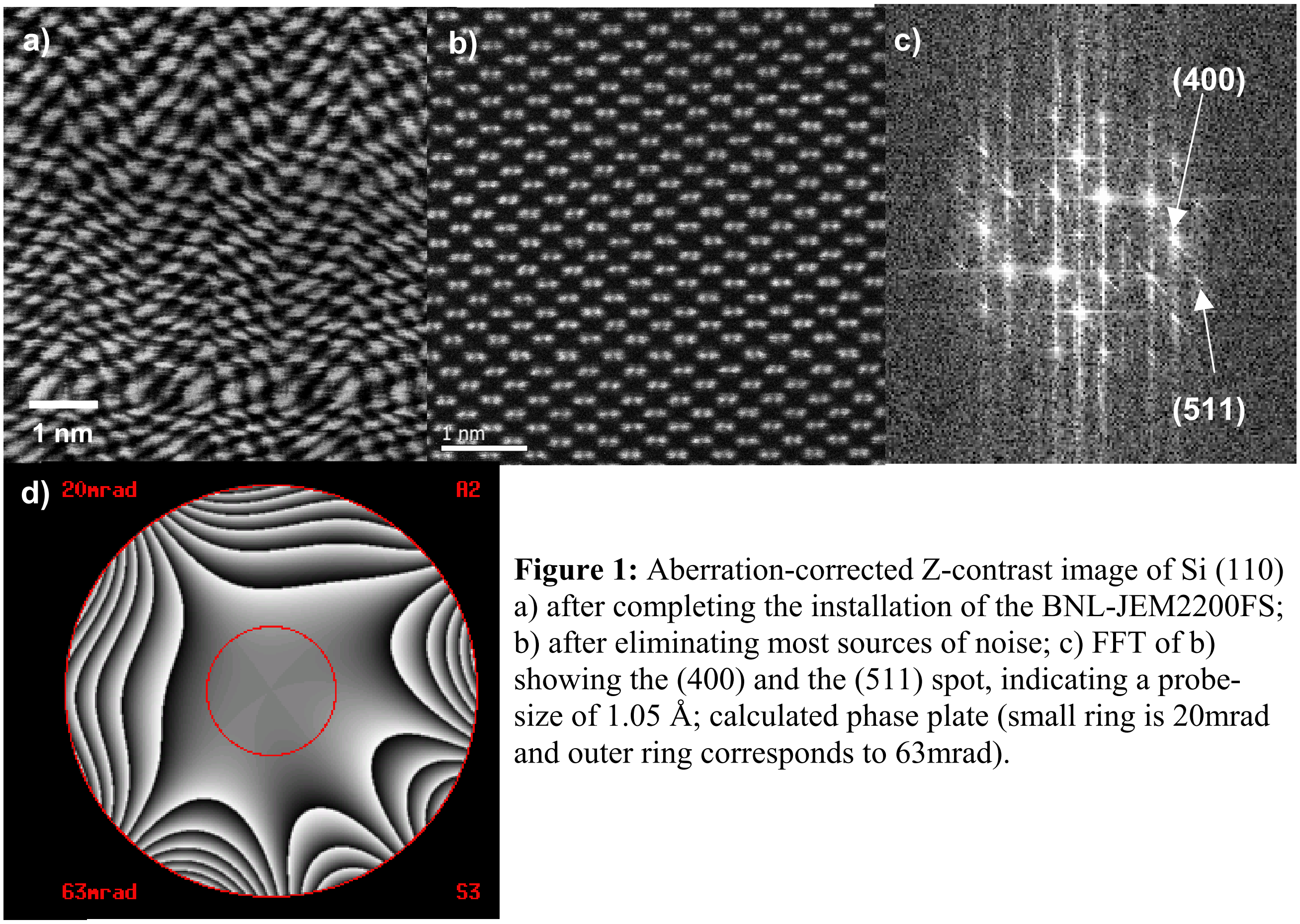

Figure 1: Aberration-corrected Z-contrast image of Si (110) a) after completing the installation of the BNL-JEM2200FS; b) after eliminating most sources of noise; c) FFT of b) showing the (400) and the (511) spot, indicating a probe-size of 1.05 Å; calculated phase plate (small ring is 20mrad and outer ring corresponds to 63mrad).

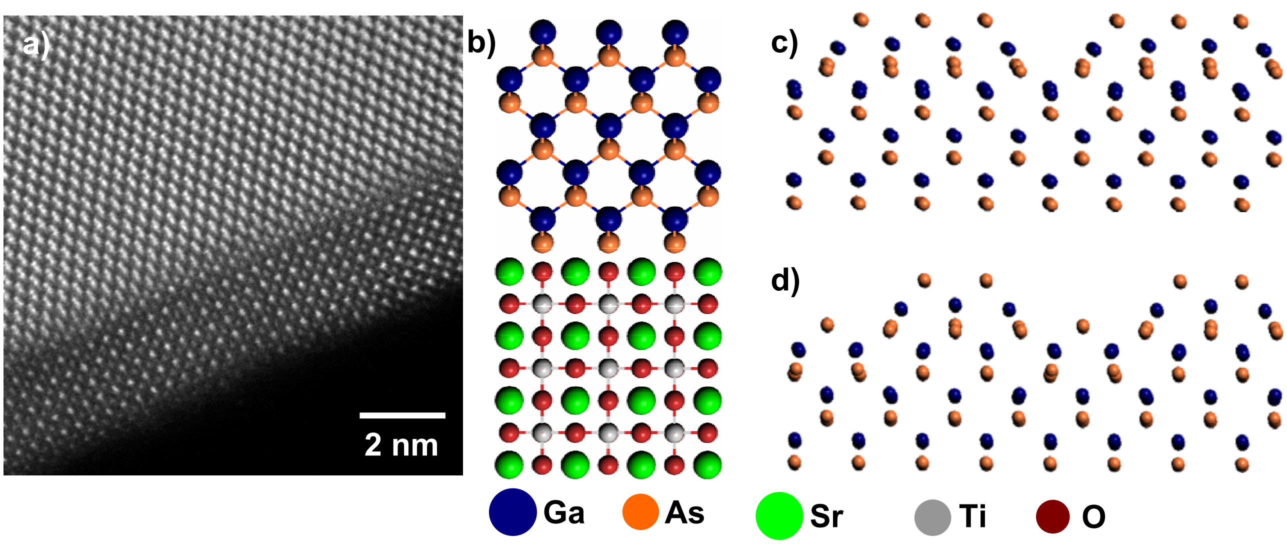

Figure 2: Atomic structure of the GaAs/$SrTiO_3$ [001] hetero-interface, a) aberration-corrected Z-contrast, b) model of the proposed interfacial structure without any surface reconstruction of the GaAs. Models of the most common 4x2 c) β and d) β2 GaAs surface reconstruction.

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