

Amplitude Contrast Imaging: High Resolution Electron Microscopy Using a Spherical and Chromatic Aberration Corrected TEM

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High-resolution transmission electron microscopy (HREM) is a powerful technique to study materials at atomic resolution. For a conventional TEM, the Scherzer defocus is typically used to maximize phase contrast and resolution. For a TEM with a spherical aberration (C_s) image corrector, Jia *et al* introduced the negative C_s imaging (NCSI) method to balance the contrast and resolution [1]. This paper shows when C_s is corrected close to zero, chromatic aberration (C_c) correction improves resolution without compromising contrast and enables amplitude-contrast imaging (ACI) in HREM.

Employing aberration correctors commercial instruments can now routinely decrease the magnitude of C_s towards zero and dramatically improve resolution. Unfortunately this also dramatically reduces the magnitude of phase contrast transfer function (PCTF) as shown in Fig. 1A. To balance resolution and phase contrast, Jia *et al* introduced the NCSI method in which a negative C_s value and a corresponding Lichte defocus are chosen to gain strong phase contrast with sufficient resolution and facilitate direct structural mapping [1]. However when C_c is uncorrected, the C_c damping envelope still limits the ultimate resolution. In an uncorrected C_c configuration, C_s corrected and uncorrected HREM images are still dominated by phase contrast as long as C_c is of significant magnitude. This is shown in Fig. 2D and 2E, which presents simulated HREM images of a $\text{CaTiO}_3/\text{BaTiO}_3$ interface using $C_s = -40 \text{ m} = -40 \text{ } \mu\text{m}$ both with $C_c = 1.5 \text{ mm}$ and show close correlation to the phase image (Fig. 2B) of the exit wave.

With C_s close to zero, we have found that C_c correction can be used to play an important role to improve resolution for both phase-contrast and amplitude-contrast HREM as a small C_c value can improve resolution without compromising phase contrast. In addition, C_c correction has an even more substantial effect on the amplitude contrast transfer function (ACTF) where C_c correction offers the possibility to exploit ACI in HREM. The green filled curve in Fig. 1C shows ACTF with small values of C_s and C_c ($C_c = 0.1 \text{ mm}$). For these conditions, the magnitude of ACTF is close to 1 over a wide range of spatial frequency nearly up to the information limit of the microscope. Under such ACI conditions (i.e. both C_s and C_c are small), the experimental image has a strong correlation with the calculated amplitude image (Fig. 2C) of the exit wave phase. An example of the correlation is illustrated in Fig. 2F, which shows the simulated image using our ACI condition.

Under ACI conditions, atomic resolution channeling contrast (ARCC) also can be realized [2]. Fig. 3 presents an amplitude contrast HREM image of a $(\text{BaTiO}_3)_4/(\text{CaTiO}_3)_4$ ferroelectric superlattice. In this image, ARCC between Ba and Ca columns is clearly observed, in which atomic columns of CaO and BaO appear bright and dark, respectively. Oxygen and Ti columns appear as bright. ARCC provides a direct and accurate measurement of the positions of oxygen columns that allows us to quantify TiO_6 octahedral tilt angles (along the [110] direction) as a function of distance from the interface. ARCC is sensitive to the mixing between Ba and Ca at the interface, allowing us to study the relationship between the mixture and octahedral tilt angles.

References:

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 [2] A. Wang, F. R. Chen, S. Van Aert, D. Van Dyck, *Ultramicroscopy* **110**, 527–534 (2010)
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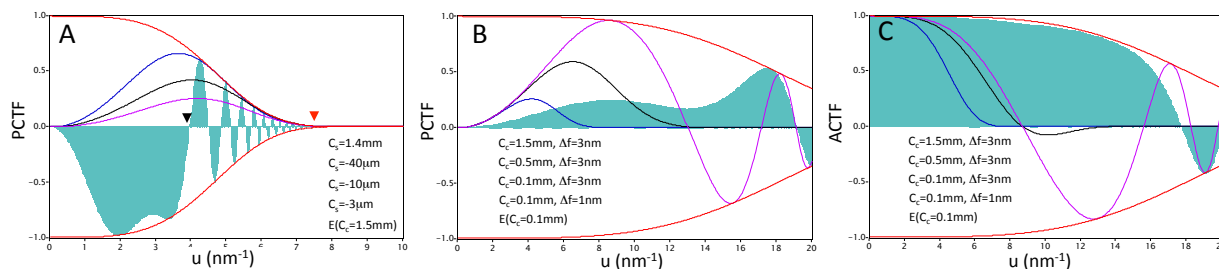


Fig. 1. (A) C_s correction improves resolution but reduces phase contrast due to the constraint of the uncorrected C_c damping envelope (red curve $C_c = 1.5$ mm). For comparison, all PCTFs are plotted at Scherzer defocus for the corresponding value of C_s . C_c correction (even just to 0.1 mm) improves both (B) PCTF and (C) ACTF up to high spatial frequencies for small C_s due to the extension of the C_c damping envelope (red curve $C_c = 0.1$ mm) to high spatial frequency. Adjusting defocus Δf from Scherzer defocus 3 nm to 1 nm improves the ACTF filled with green in (C) to close to 1 over a wide range of spatial frequency up to the information limit of the microscope.

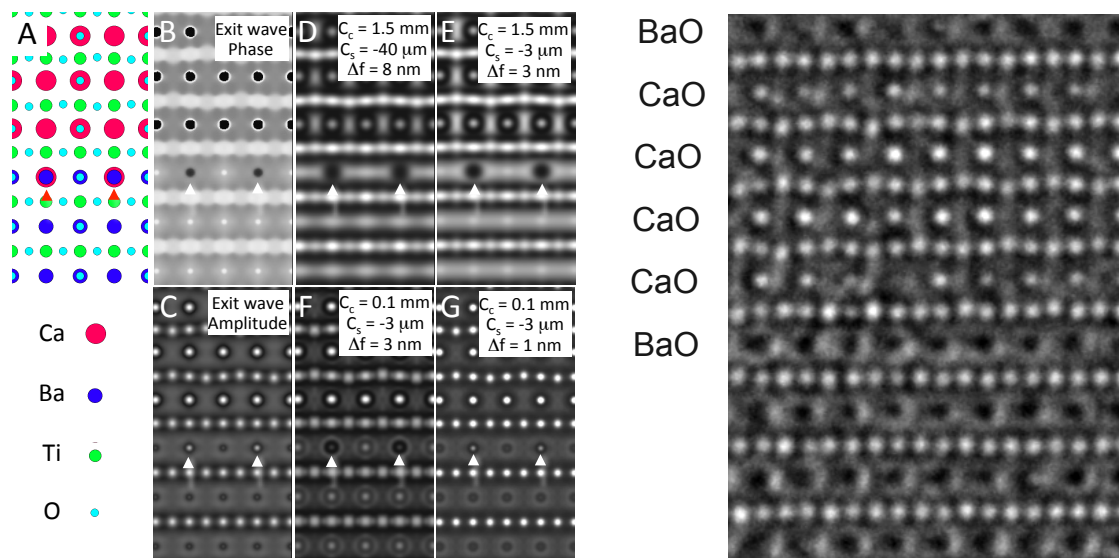


Fig. 2. Simulated images of the $\text{CaTiO}_3/\text{BaTiO}_3$ interface demonstrating that correction of C_s and C_c enables amplitude contrast HREM. (A) Atomic arrangement along [110]. (B) Phase image and (C) amplitude image of exit wave of a 9 nm thick sample. When C_c is uncorrected $C_c=1.5$ mm), both simulated images using (D) $C_s = -40$ μm and (E) $C_s = -3$ μm show close correlation to phase image of the exit wave in (B). When C_c is corrected from (E) $C_c=1.5$ mm to (F) $C_c=0.1$ mm, simulated image in (F) shows close correlation to the amplitude image of the exit wave in (C). Adjusting defocus further improves the amplitude contrast in (G).

Fig. 3 Experimental image of a $\text{CaTiO}_3/\text{BaTiO}_3$ superlattice along [110] with an amplitude contrast HREM imaging condition of $C_s = 3$ μm , $C_c = 1$ μm . Atom columns of CaO, Ti, and O in this image appear as bright dots on a grey background. Atom columns of BaO appear darker. The image shows close correlation to the amplitude image of the exit wave.