एक बहु-घटक प्रणाली के विपथन संशोधित STEM-iDPC कंट्रास्ट में स्पष्ट विसंगतियों की व्याख्या

Understanding Apparent Anomalies in Aberration Corrected STEM-iDPC contrast of a Multicomponent System

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Integrated Differential Phase Contrast (iDPC) has emerged as one of the most useful detectors in recent times, owing to its ability to simultaneously image both high- and low-Z elements. It is an advanced STEM technique that creates potential maps of thin samples by integrating DPC signals from segmented detectors [1]. The method typically uses a quadrant detector (or multi-sector detector) to measure the center-of-mass (COM) of the convergent beam electron diffraction pattern, which is then integrated to produce a scalar phase image. iDPC provides linear phase contrast imaging with low dose efficiency, making it particularly suitable for beam-sensitive materials. The technique excels at imaging light elements next to heavy ones, even at low electron doses. Unlike ABF, iDPC produces images where light elements appear with bright contrast against a dark background. Advanced implementations use multi-sector detectors (8, 12, or even 48 segments) instead of simple quadrant detectors to achieve more isotropic contrast transfer functions and improve image quality. This enhancement reduce anisotropy artifacts and provide better contrast and resolution, especially for thick samples. iDPC-STEM produces an image contrast that is proportional to the projected electrostatic potential [2], enabling high-resolution visualization of both light and heavy elements, where the contrast is directly proportional to the atomic number Z [3]. However, this narrative is only valid under certain conditions, as will be demonstrated here.

Fig.1 shows the STEM-iDPC images acquired along the [100] and [001] ZA in $(Fe,Cr)_2B$ of a melt-cast ferrite–boride composite [4 – 6]. It is interesting to note that the Fe/Cr and B atomic columns appeared with nearly equal intensities along [001] in contrast to [100], where the intensity was proportional to the Z of the atom. The approach that iDPC intensities are proportional to Z implicitly assumes that iDPC intensity differences directly reflect projected atomic potential. This treatment leaves a key ambiguity: why did the Fe-B contrast in [001] differ so markedly from the [100]. The ambiguity arises because of the influence of imaging conditions, such as specimen thickness, defocus, and zone-axis-dependent dynamical scattering, as discussed below.

The iDPC contrast transfer function (CTF), derived in detail by Lazic et al. [7] and evaluated in Liang et al. [8], governs how different spatial frequencies are transferred to the image and is extremely sensitive to defocus, specimen thickness, accelerating voltage, convergence angle, collection angle, sample tilt, and electron dose. For thin samples, the iDPC signal is approximately proportional to the projected potential, making the intensity roughly proportional to atomic number. For thicker samples, however, multiple scattering, dechanneling, and the anisotropy of the CTF can drastically alter contrast, even reversing the relative intensities of atomic species. The experimental thickness for the region studied here, determined from zero-loss EELS analysis, was approximately 20 nm and 30 nm for [100] and [001] ZA samples, respectively. The iDPC images were acquired at a nominal defocus of -4 nm. Multislice simulations were carried out using Dr. Probe software to interpret the experimental contrast behavior. The simulation series varied defocus from -10 nm to +4 nm in 2 nm steps and thickness from ~0.5 nm to ~50 nm. Fig.2 shows the simulated iDPC contrast variation for (a) [100] and (b) [001], respectively, across the full defocus-thickness space.

Along the [100] direction, the channeling of the probe along Fe/Cr columns is less perturbed by neighboring B columns. In the simulated contrast maps, shown in (a), even at t=20 nm, the Fe/Cr-B intensity difference remains appreciable over a wide range of defocus values. This thinner sample remains closer to the single-scattering regime, so iDPC intensities retain more of their monotonic Z-dependence. Along the [001] direction, the projection geometry places B columns in closer lateral proximity to Fe/Cr columns, thereby increasing the likelihood of dynamical scattering between them. This effect is pronounced at intermediate thicknesses (20-40 nm), as shown in Fig.2(b), where multiple scattering redistributes intensity between columns. In Fig.2(b), the contrast maps reveal a plateau in the defocus-thickness space where the Fe/Cr and B intensities converge.

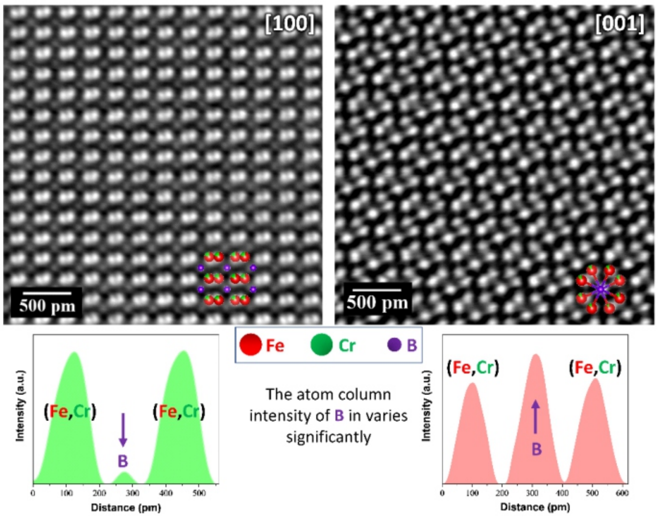

Fig.1: Quantitative comparison of iDPC-STEM contrast between Fe/Cr and B atom columns for (Fe,Cr)2B along [100] and [001].

The experimental defocus (-4 nm) and thickness (~30 nm) sit in this plateau, explaining the observed similarity in intensity.

Therefore, it is clear that an intriguing interplay between sample thickness and defocus in iDPC imaging is responsible for relative intensities of higher vis-à-vis lower Z elements in a multicomponent system.

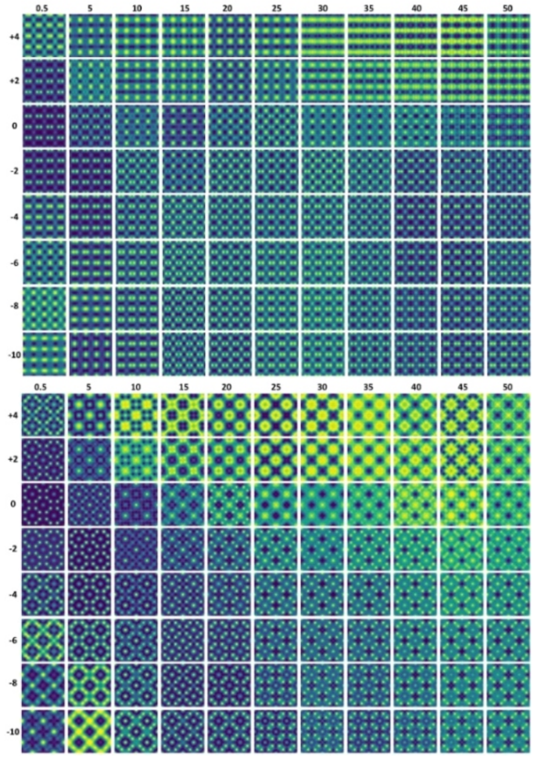

Fig.2: Simulated iDPC-STEM contrast for $(Fe,Cr)_2B$ along (left) [100], and (right) [001] as a function of defocus (vertical axis, nm) and specimen thickness (horizontal axis, nm).