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Challenges of Oversimplifying Z-contrast in Atomic Resolution ADF-STEM

Ryan J. Wu[1], Michael L. Odlyzko[1], K. Andre Mkhoyan[1]

[1.] Department of Chemical Engineering and Material Science, University of Minnesota, MN, USA

Using thickness or atomic number (Z) to interpret variations in the intensity of atomic columns has been a trademark of annular dark-field scanning transmission electron microscopy (ADF-STEM) images. As widely accepted theory, higher Z elements, in general, show increase scattering compared to lower Z elements [1]. For experiments involving a predetermined binary compound (BN, GaAS, AlN, etc), Z contrast, alone, is often times enough to conclude the chemical identity of an atomic column. This interpretation is accurate under ideal electron beam behavior where the STEM probe propagates with the majority, if not all, of its intensity along a single atomic column. However, Odlyzko [2], among others, established electron beam channeling can spatially spread the intensity of a propagating electron beam beyond a single atomic column. Under these conditions, even when a STEM probe is localized to an atomic column, a non-negligible amount of probe intensity could transfer to neighboring columns. This behavior makes image interpretation more complex, and oversimplifying conventional Z-contrast can potentially lead to wrong conclusions from ADF-STEM images.

In this work, multislice simulations [3] were used to analyze the reliability of Z-contrast in ADF-STEM imaging for binary compounds with similar Z where intensity transfer to neighboring columns is known to occur [1,4,5]. Figure 1 shows simulated ADF-STEM images of [110] GaAs at 3 different thicknesses. At 5 nm where the electron beam still maintains its initial spatial intensity distribution, the Ga and As atomic columns obey conventional Z-contrast rules, where the higher Z element shows higher intensity. At an intermediate thickness (35 nm), the intensity of the Ga and As atoms appear equal which indicates a partial amount of propagating beam intensity has shifted from one atomic column to another. Finally at 50 nm, the Ga atomic column now appears brighter than the As atomic column. This defies conventional Z-contrast interpretations where one would believe the Ga atom is the As atom when, in fact, it is not. Figure 2 shows simulated ADF-STEM images of [110] c-BN similar to GaAs in the previous figure. Here, at the intermediate thickness (30 nm), the intensity of B atoms almost resembles the N atoms. However, at later thicknesses, the intensity does not flip as in the GaAs case. Thus, the presence and severity of this intensity transfer behavior is not prevalent across all binary materials with similar Z. Simulations show that initial electron probe parameters such as the voltage and convergence angle can affect its channeling behavior and hence its ability to transfer intensity. Furthermore, the distance between neighboring columns also affects the magnitude of the intensity transfer. In light of the results, decoupling these effects is necessary to correctly interpret ADF-STEM images even for simple binary compounds [6].

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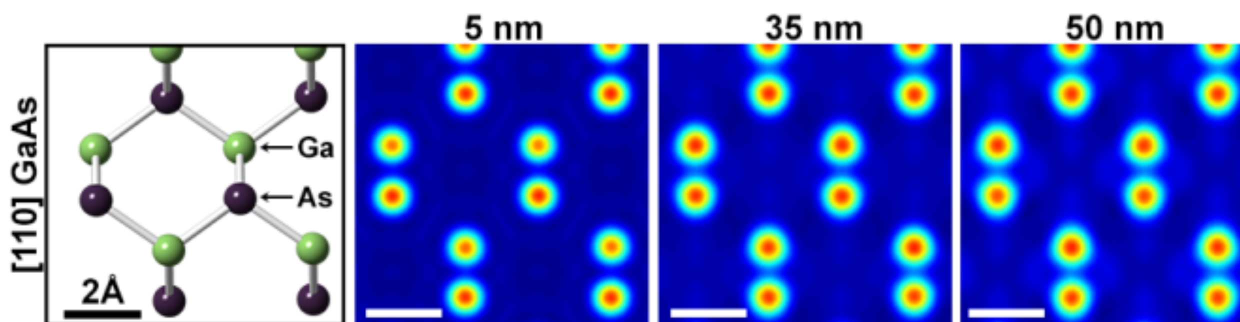

Figure 1. Simulated ADF-STEM images of gallium arsenide at various thicknesses. From left to right: ball-and-stick model of [110] GaAs; 5 nm thick GaAs; 35 nm thick GaAs; 50 nm thick GaAs. Each image is individually normalized from 0 to 1.

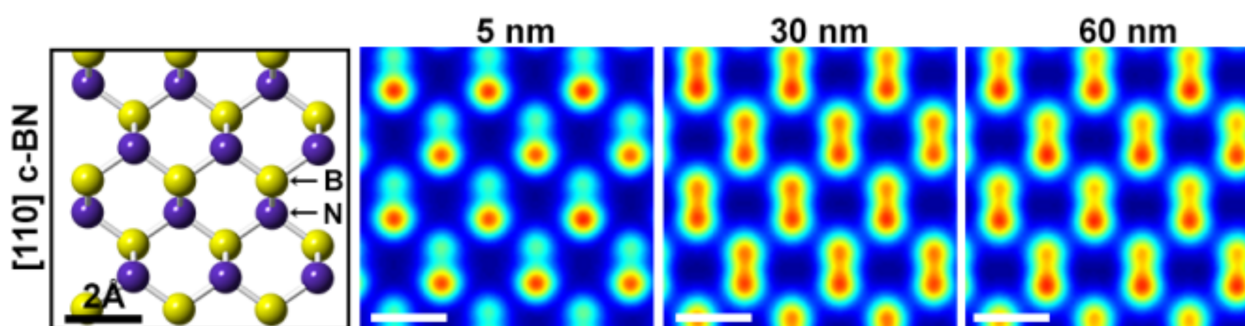

Figure 2. Simulated ADF-STEM images of cubic-boron nitride at various thicknesses. From left to right: ball-and-stick model of [110] c-BN; 5 nm thick c-BN; 30 nm thick c-BN; 60 nm thick c-BN. Each image is individually normalized from 0 to 1.

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