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Interfacial Atomic Number Contrast in Thick Samples

Aniruddha Dutta[1] and Helge Heinrich[1]

[1] Advanced Material Processing & Analysis Center (AMPAC), Department of Physics, Department of Physics, University of Central Florida, Orlando, FL, USA.

A quantitative method to simulate the electron scattering at the interface of two material layers in thick samples is presented here. The samples are analyzed by Scanning Transmission Electron Microscopy (STEM) in a Tecnai F30 using a High Angle Annular Dark-Field (HAADF) detector with a collection range 55 mrad to 245 mrad. At the interface of a high-density and low-density material an increase in the HAADF signal for thick TEM samples can be observed. We report here the simulated HAADF detector intensity across the interface of two materials using Python programming language and its comparison with experimental results.

The electron atomic scattering factor f^e(s) for a complex potential is given by:

$$f^e\left(s_i\right)=\sum_{i=1}^{5} a_i \exp\left(b_i s_i^{\,2}\right) \tag{1}$$

where a_i and b_i are scattering parameters [1, 2]. $s=\dfrac{\sin\theta}{\lambda}$ where θ is the Bragg angle. The scattering cross section is given by:

$$f^b=\left[\frac{2\pi\gamma mq}{h^2}\right]f^e \tag{2}$$

where γ is the relativistic correction [3-5]. Samples from Focused Ion Beam (FIB) processing can be relatively thick (> 100 nm). In the current study we prepared a wedge-shaped sample with a FEI 200 TEM FIB system, where the sample thickness increases with distance from one edge. When the electron beam is focused at the interface of a high- and low-density material, electrons get scattered in both materials at high angles. For an electron beam entering near the interface but within the high-density material a fraction of the electrons exit the high-density material and get scattered into the neighboring low-density material at high angles thus suffering less absorption before reaching the detector. We therefore see increased intensities at the interface as shown in Fig. 1.

The program uses a random scattering approach for a large number of electrons, where we calculate the path of individual electrons through the material. A standard multislice method cannot be applied for samples much thicker than 100 nm as the high scattering angles used here require extremely large multislice frames larger than 2^{15}x2^{15} pixels. The electrons suffer multiple scattering before they are detected by the HAADF-STEM detector after traversing through a sample thickness of several 100 nm. Fig. 2 plots the HAADF-STEM detector signal with respect to the position on the interface of W and SiO_2. As the simulated electron beam is scanned across the interface, the HAADF-STEM detector collects the fraction of scattered electrons (detector intensity normalized) from the left to the right where zero on the x-axis represents the interface of the two materials. As shown in Fig. 2 just to the right of the interface there is about four times in increase in the detector signal. This is in accordance with the experiments as a fraction of electrons goes from high-density material (high absorption) to the low-density material (low absorption).

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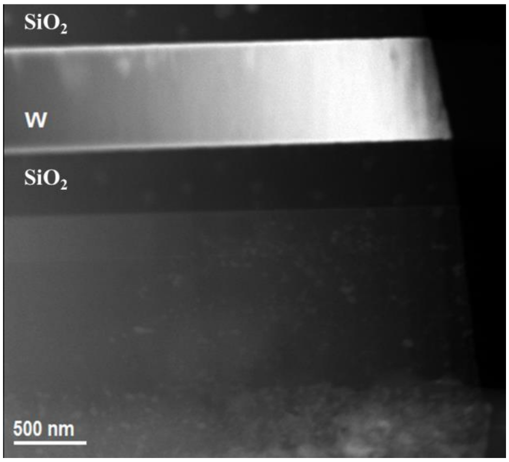

Figure 1. HAADF-STEM micrograph showing the increase in signal near the interface of a high and low density material (here W and SiO_2).

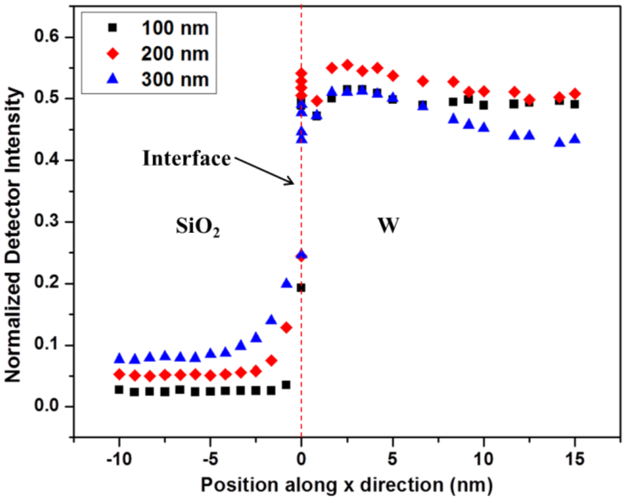

Figure 2. Simulated HAADF-STEM detector signal across the interface of W and SiO_2.