doi:10.1017/S1431927613006259
Microsc. Microanal. 19 (Suppl 2), 2013

Simulation of incoherent scattering in High-Angle Annular Dark-Field Scanning Electron Microscopy

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A quantitative method to simulate the electron scattering intensities in Scanning Transmission Electron Microscopy (STEM) for High-Angle Annular Dark-Field (HAADF) detectors is presented. A HAADF detector in a 300 kV transmission electron microscope collects electrons scattered to high angles with its intensity nearly proportional to the sample thickness and increasing with atomic number. Multislice simulations in Python 2.7 are used to calculate the scattering cross sections and the final intensity of the electron beam after multiple scattering events and for comparison with experimental results.

For a complex optical potential the electron atomic scattering factor $f^e(s)$ consists of a real and an imaginary part where a sum of n Gaussian is applied to fit the following equation:

$$f^e(s_i) = \sum_{i=1}^{n} a_i \, exp(b_i s_i^2) \qquad (1)$$

where a_i and b_i are fitting parameters [1]. In (1), s = sinθ/λ, where θ is the angle of scattering and λ is the wavelength of the incident electron. For several elements the scattering cross sections were calculated keeping the HAADF detector range between 55 mrad and 245 mrad. The total scattering factor for all values of θ from 0 to π rad is given by:

$$f^b = \left[\frac{2\pi\gamma mq}{h^2}\right] f^e \quad \text{[2-3]} \qquad (2)$$

where $\gamma = 1 + \frac{qv}{mc^2}$ is the relativistic correction.

For incoherent scattering the intensity of the electron beam after first layer scattering is given by:

$$I_1 = (f^b)^2 t\rho \qquad (3)$$

where ρ is the density of aluminum and t is the thickness of the layer. The electrons hitting the sample perpendicularly suffer no scattering and the intensity of the beam has been considered as unity. The intensity values for aluminum sample at different angle of scattering of the electrons is calculated for increasing thickness step and matched with the experimental values of the fraction of scattered electrons per nm sample thickness according to the following equation:

$$I_2 = (f^b)^2 t\rho d\theta \qquad (4)$$

Our Python program computes the relative intensity with respect to the intensity of the electron beam at the center of the sample which takes values for the detector area only.

The HAADF-STEM intensity values are shown in Fig 1. taking into account the absorption taking place. The algorithm calculates the HAADF intensity as a function of sample thickness.

References:

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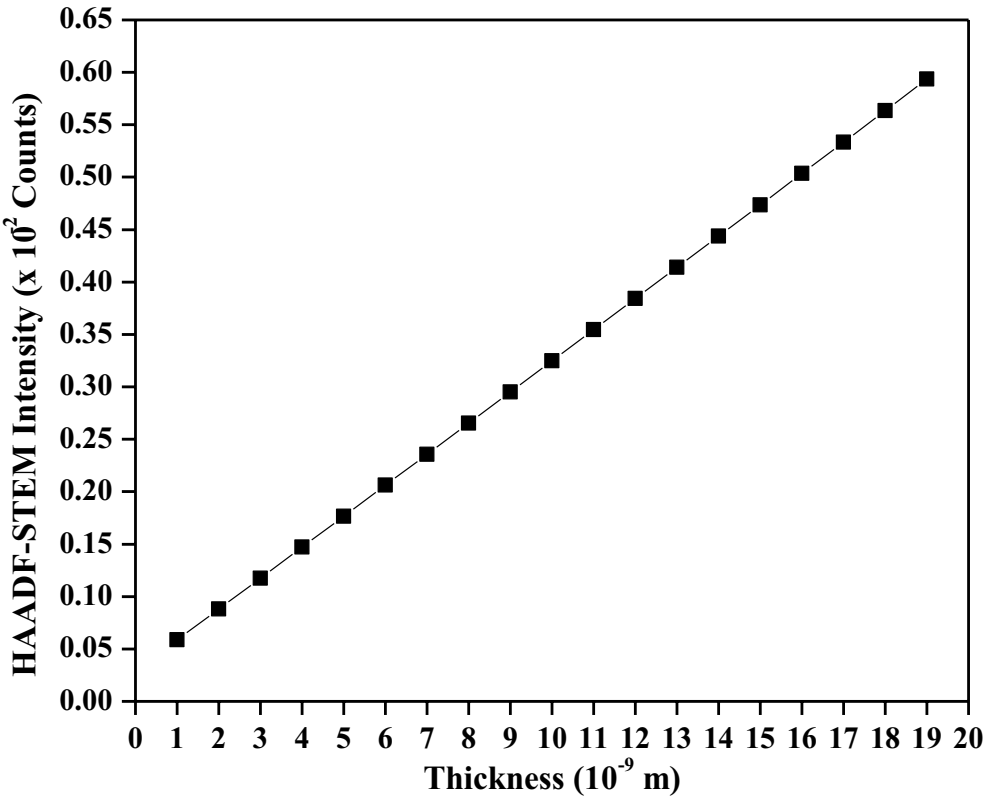

Figure 1. HAADF-STEM intensity as a function of sample thickness for aluminum

https://doi.org/10.1017/S1431927613006259 Published online by Cambridge University Press