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A universal equation for computing the beam broadening of incident electrons in thin films

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ABSTRACT

A universal equation for computing the beam broadening of incident electrons in thin films is presented. This equation is based on the concepts of anomalous diffusion with the Hurst exponent H. When the thickness to elastic mean free path ratio, t/λ, is greater than 1, the Hurst exponent goes to 0.5 and this random walk behavior leads to the Goldstein et al. [1] beam broadening equation when non-relativistic screened Rutherford elastic cross-sections are used. When $t/\lambda \ll 1$, the lack of elastic collisions for the electron trajectories gives an H exponent of 1 and a different beam broadening equation is obtained. A general equation to compute the beam broadening that takes into account the variation of H with t/λ is presented and this equation was fitted and validated with Monte Carlo simulations of electron trajectories in thin films.

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1. Introduction

Computing the beam broadening of transmitted electrons is needed for determining the spatial resolution of X-ray microanalysis in the transmission electron microscope (TEM) and also in the low variable pressure scanning electron microscope (VP-SEM). As seen in Fig. 1 in a TEM thin film specimen, the incident beam diameter is smaller than the phase B to be analysed. Because of the beam broadening in this specimen, the electrons scatter in the phase A and the chemical composition obtained through EDS, for example, will be between those of A and B and the exact value of B cannot be measured. It is therefore important to estimate the beam broadening when quantitative analyses are performed in electron microscopy. The spatial resolution of quantitative analysis in thin films is therefore limited by the beam broadening. In the case of the VP-SEM, this is the beam broadening in the gas above the specimen which can also degrade the spatial resolution.

The diameter of the transmitted electrons, R_{max} depends on the incident beam diameter d and of the broadening of the electrons in the specimen because of scattering events. The beam broadening for a beam diameter equal to zero is represented by b. The convention of taking the values of d and b that correspond to 90% of the incident and scattered electrons is typically used. Assuming that the incident beam diameter and the beam broadening are described by a Gaussian distribution, R_{max} can be computed by this equation

$$R_{max}=\sqrt{d^2+b^2} \quad (1)$$

With the advent of field emission transmission electron microscopes with spherical aberration correctors, a probe diameter of about 0.1 nm can be obtained routinely. The spatial resolution of EDS X-ray microanalysis becomes therefore limited by the beam broadening in the specimen, as seen in Eq. (1). The beam broadening is commonly evaluated with the single scattering equation derived by Goldstein et al. [1] even if it could be computed by Monte Carlo simulations [2]. Fig. 2 shows the geometry used in their model where they assume that a single elastic collision always occurs at the middle of the specimen with an effective collision angle θ^*. They obtained the following equation for b:

$$b=625\frac{Z}{E_0}\sqrt{\frac{\rho}{A}}\,t^{3/2}(\text{cm}) \quad (2)$$

where Z is the atomic number of the thin film of thickness t, in cm, ρ is the mass density, in g/cm^3 , A is the atomic weight, in g/mol, of the thin film and E_0 is the energy of the incident electrons, in keV. The single scattering model of Goldstein et al. [1] predicts that b scales with $t^{3/2}$. Moreover, Eq. (2) can be rewritten in order to obtain a universal curve, as predicted by their model

$$\frac{b}{625\frac{Z}{E_0}\sqrt{\frac{\rho}{A}}}=t^{3/2} \quad (3)$$

In order to validate the behavior predicted by Eq. (3), Monte Carlo simulations, described later in this paper, were performed for 1,000,000 electron trajectories in thin films of C, Al, Fe, Ag, and Au for thicknesses ranging between 10 and 200 nm and E_0 equal to

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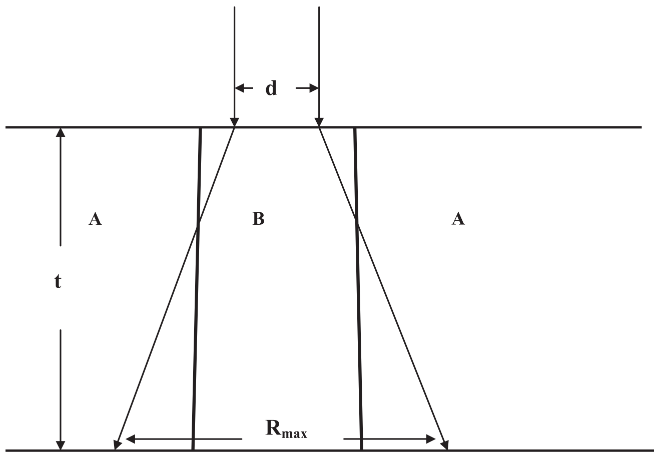

Fig. 1. Diameter of the transmitted electrons, R_{max}, after the broadening of an incident beam of diameter d inside of a thin film of thickness t. The incident beam diameter is smaller than the phase B to be analysed. Because of the beam broadening in this specimen, the electrons scatter in the phase A and the chemical composition obtained through EDS, for example, will be between those of A and B and the exact value of B cannot be measured.

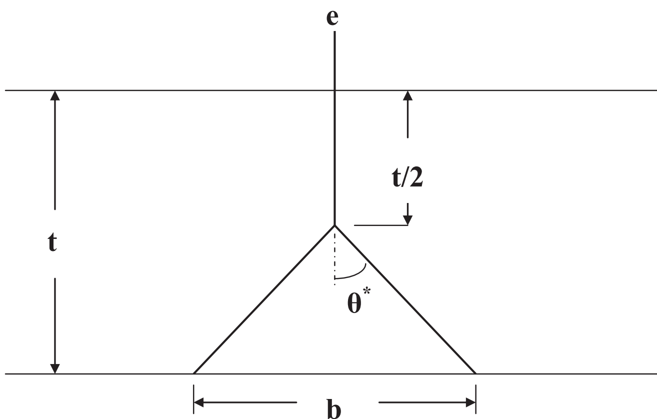

Fig. 2. Geometry used in the scattering model of Goldstein et al. [1] where they assumed that a single elastic collision always occurs at the middle of the specimen with an effective scattering angle θ^*.

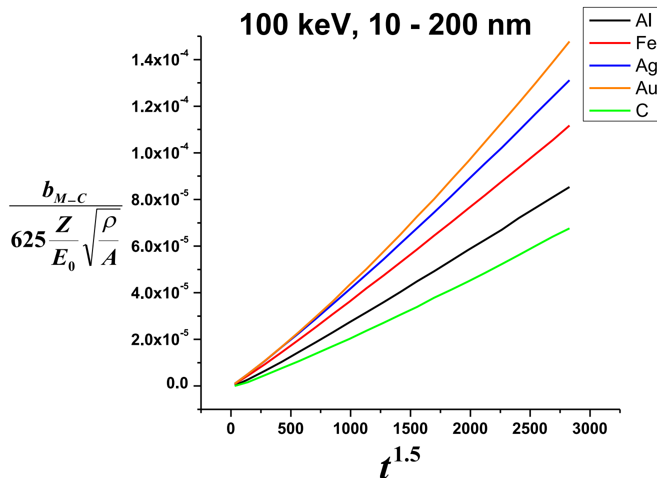

Fig. 3. b, Normalized, as shown in Eq. (3) as a function of $t^{3/2}$. b was computed with Monte Carlo simulations of 1,000,000 electron trajectories [5].

100 keV. Fig. 3 shows b obtained by Monte Carlo, normalized as shown in Eq. (3), as a function of $t^{3/2}$. The universal behavior, predicted by Eq. (3) is not observed, which indicates that the validity of the single scattering model of Goldstein et al. [1] can be questioned and/or that the scaling given by Eq. (3) is not the right one. Moreover, as seen in Fig. 2, $b = t \tan \theta^*$. Since the energy loss does not change significantly in a thin foil, the effective scattering angle θ^* is constant. Also, θ^* is small for electron energies above 10 keV and therefore, $b \cong \theta^* t$. A single scattering model which assumes that a collision always occurs inside a specimen should give a linear dependence on the beam broadening with the specimen thickness, which is not the case with the Goldstein et al. [1] model. Moreover, the single scattering event does not always occur in the specimen because the probability of collisions inside the specimen follows Poisson's statistics and is smaller than one for specimens with thicknesses smaller than the elastic mean free path. In this paper, a new equation for computing the beam broadening is proposed that is shown to reduce to the Goldstein equation in the plural scattering regime. This is important because the Goldstein equation is known to work very well in the plural scattering regime [3,4], i.e. the $t^{3/2}$ dependence is valid for random walk behavior or a diffusion regime. This new beam broadening equation is simpler and more physical than another beam broadening equation previously derived by one of the authors [5,6]. The derivation of the previous equation is performed again in Appendix B of this paper with more detail. The new equation presented in this paper was fitted with Monte Carlo simulations to give a workable equation. This new equation bears similarities with the beam scattering equation proposed by Cliff and Lorimer [7] but has a different variation of the thickness exponent with specimen thickness since the new equation accounts for the probability of scattering at small thicknesses that leads to another limiting equation. A simple parameterization is presented and compared with elaborate Monte Carlo simulations of electron scattering in thin films of various thicknesses and electron beam energies for materials of different compositions.

2. New scattering model

2.1. Derivation of the general expression

A general equation must be valid in the case of single scattering as well as multiple scattering, i.e., as the thickness to the elastic mean free path ratio, t/λ, goes from 0 to 25, the multiple scattering regime [3]. When many collisions occur in the specimen, the beam broadening, b, is twice the sum of all the projected distances, r_i, in the exit plane of the thin foil of each individual collision, as seen in Fig. 4. Therefore

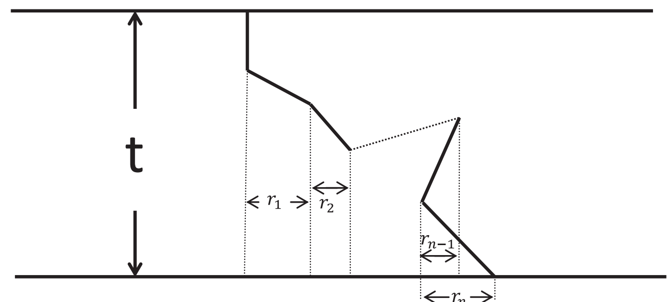

Fig. 4. Projected distances, r_i, in the exit plane of the thin foil of each individual collision.

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