DOI: 10.1017/S1431927605510675
Microsc Microanal 11(Suppl 2), 2005

On the Development of Phi-Ro-Z Models with Physical Meaning using Monte Carlo Simulations

Raynald Gauvin

Department of Mining, Metals & Materials Engineering, McGill University, 3610 University Street, Montréal, Québec, Canada, H3A 2B2

Quantitative x-ray microanalysis in the electron microprobe or in the scanning electron microscope is based on the following equation:

$$\frac{C_i}{C_{(i)}} = [ZAF]_i \frac{I_i}{I_{(i)}} \quad (1)$$

where I_i is the net intensity of the characteristic line of element i measured in the analyzed specimen of composition C_i, $I_{(i)}$ is the net intensity of the same characteristic line of the same element measured on a standard of known composition $C_{(i)}$ and $[ZAF]_i$ are the correction factors needed to solve equation (1). The modern approach is based on the use of $\varphi(\rho z)$ models to compute the Z and A factors. The first successful model was developed by Packwood & Brown [1] and later improved by Bastin & Heijligers [2]. This model is based on a Gaussian function to model the second part of the $\varphi(\rho z)$ curve, being justified by the fact that electrons reach a random walk behavior when they scatter into a solid. Figure [1] shows $\ln(\varphi(\rho z))$ versus $(\rho z)^2$ for the M_5 shell of Au and for the K shell of C obtained from Monte Carlo simulations in bulk Au and C respectively at 20 keV. A Gaussian behavior is justified for Au but not for C since a random walk behavior can not be obtained for that element [3]. Therefore, others models are needed for light elements despite the success of some models based on two parabolas [4] and on two exponential functions [5]. The success of these later models is due to extensive fitting of the parameters of these $\varphi(\rho z)$ models, especially for light elements. In order to obtain more reliable physical parameters for a $\varphi(\rho z)$ model that describes x-ray emission from a light matrix, a model with more physical meaning must be developed. In that context, we must start with an exact equation for the $\varphi(\rho z)$ curve for a pure element [6]:

$$\varphi(\rho z) = n(\rho z)\frac{Q(E(\rho z))}{Q(E_0)}\langle \sec(\theta)(\rho z)\rangle \quad (2).$$

Figure [2] shows a comparison of a Monte Carlo simulated $\varphi(\rho z)$ curve for C K at 20 keV and with this computed with equation (2) with the 3 functions derived with the same simulation. Clearly, the agreement is excellent and a real physical $\varphi(\rho z)$ model should be based on equation (2).

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Figure [1]

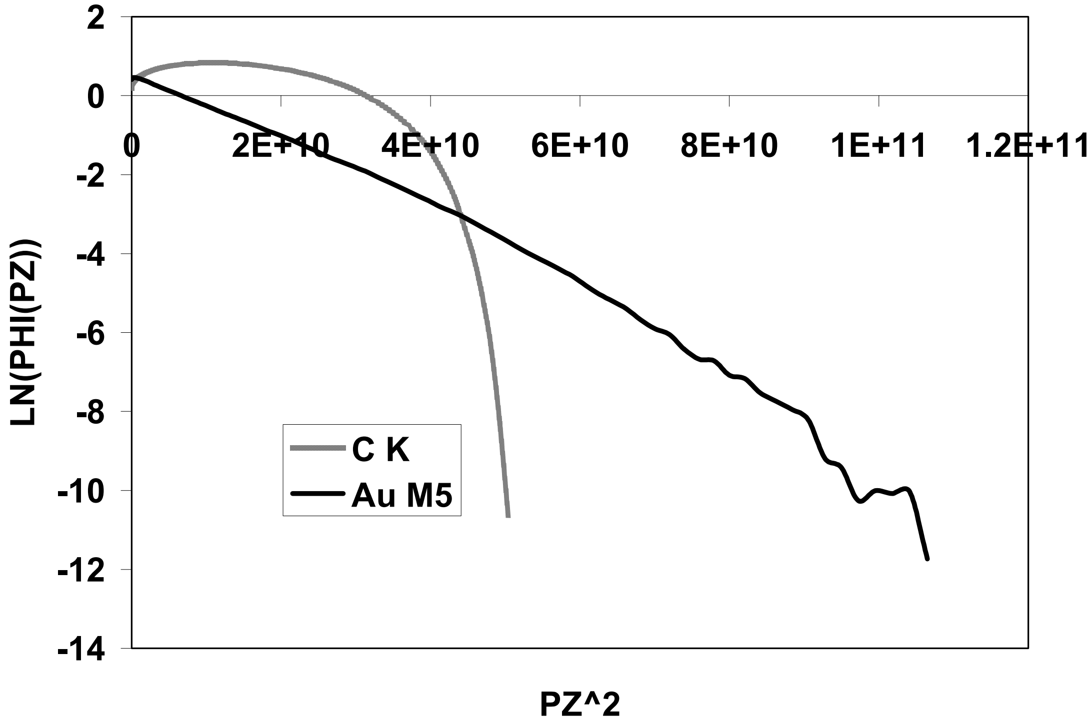
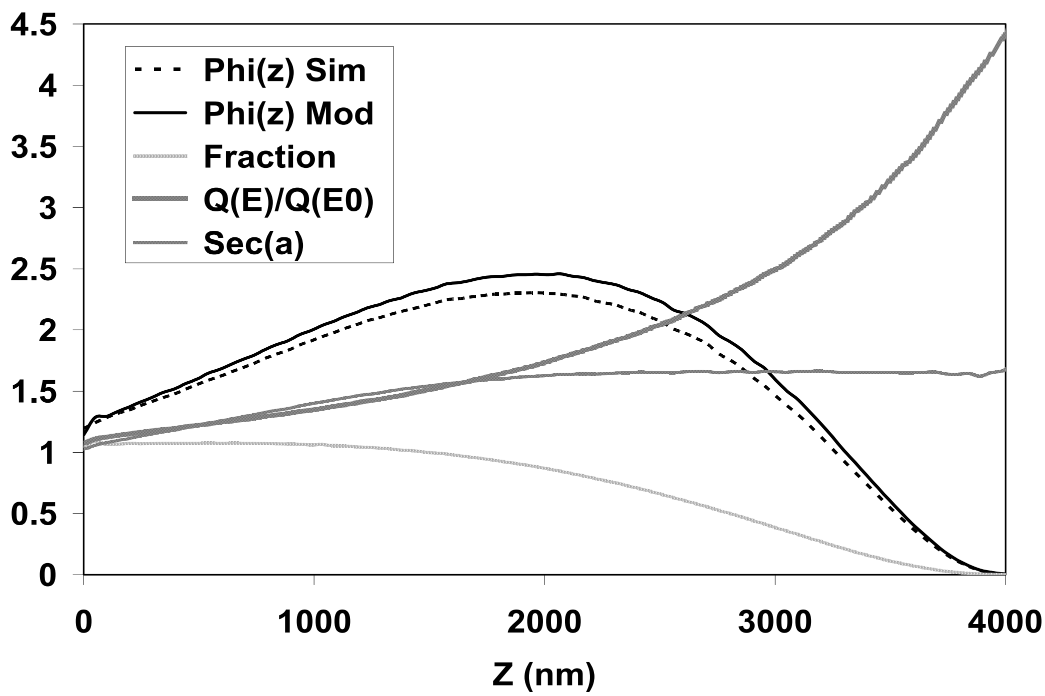


Figure [2]



https://doi.org/10.1017/S1431927605510675 Published online by Cambridge University Press