A Monte Carlo Calculation of Backscattering Factors for Compounds

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With the progression of nowadays technological innovations, the significance of Auger electron spectroscopy (AES) as an instrument for analyzing the chemical composition of surfaces and films has been increasingly recognized. In the field of quantitative surface analysis by AES the importance of a critical physical factor for composition correction, namely the backscattering factor, cannot be overstated. This factor noted as $1+r$ accounts for the percentage contribution of backscattered electrons, in addition to the primary electrons, to the generation of Auger signal electrons within the surface vicinity. The factor also approximates to $\phi(\rho z=0)$ in value in electron beam microanalysis for x-ray generation. It depends on many experimental factors including primary energy, incident angle, the sample chemical composition and the inner-shell of ionization for related Auger transition. Therefore, it has presented a considerable challenge for experimental determination and, consequently, the experimental data of backscattering factor are sparse and typically cater to a particular specimen and an inner-shell.

On the other hand, the theoretical modeling has emerged as the predominant approach for deriving this factor. Ichimura and Shimizu have pioneered a Monte Carlo method for the theoretical calculation of the backscattering factor and performed systematic calculations for over 25 materials including pure elements, compounds and alloys [1]. The calculated data were then later fitted into an empirical formula for practical use. While their calculation was based on an old definition of backscattering factor. However, twenty years later Jablonski has presented a generalized definition of $1+r$ through the excitation depth distribution function and the emission depth distribution function [2]. The new definition leads to the modified $1+r$ value, which can be even less than unity at low voltage ratio (i.e. the ratio of incident energy to ionization energy). Moreover, the configuration of the detection apparatus can be factored into the computation via the solid angle and orientation parameters. Given the multi-parameter dependency, devising a simple empirical formula becomes formidable. For this, Zeng *et al* have employed an improved Monte Carlo simulation approach to calculate backscattering factor for 28 elemental substances based on the new definition [3]. Both the configuration geometry of concentric hemispherical analyzer and the cylindrical mirror analyzer for Auger electron detection are considered. This work for elemental solids has laid a ground for constructing a database of backscattering factor. In the calculation both the incident electron trajectories and Auger electron trajectories are separately traced to derived the excitation depth distribution function and the emission depth distribution function, respectively.

The present work then aims to further extend the calculation to compound solids to enrich the existing database. We have calculated the backscatter factors for the O KLL transition of five oxides: Cu_2O, CuO,

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HfO_2, In_2O_3 and ZrO_2. Fig. 1 shows the results for ZrO_2, displaying the data selected for specific condition of incident angle, primary energy and detection angle.

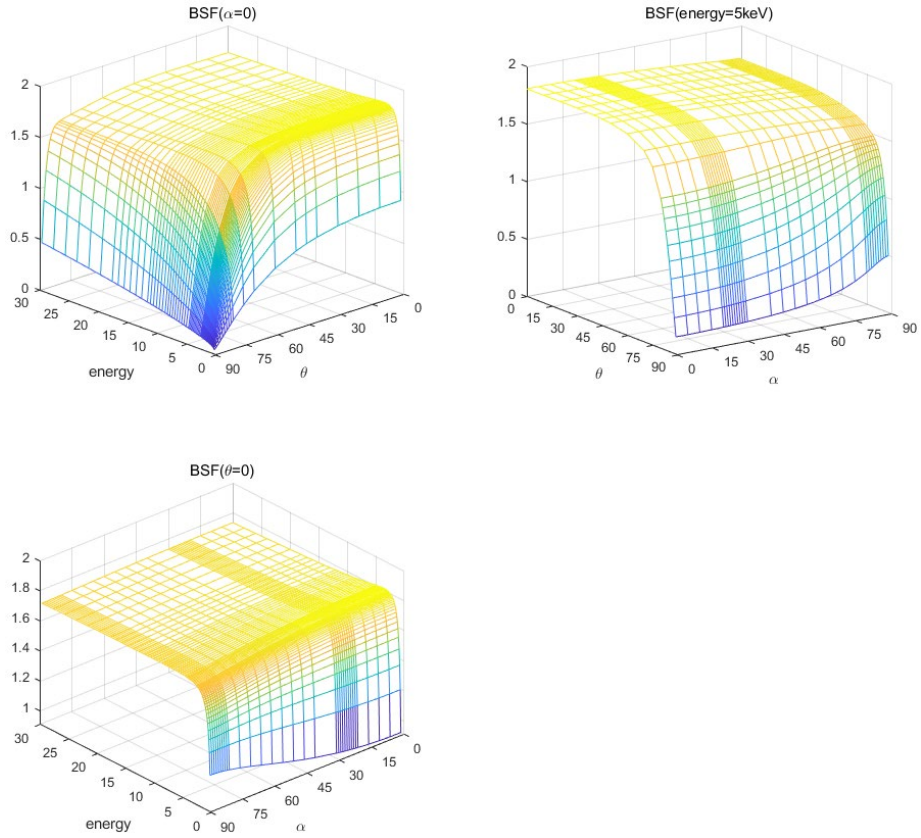

Figure 1. The dependence of the calculated backscattering factor on primary energy, incident angle and detection angle for O KLL transition of ZrO_2.

Keywords： backscattering factor; Monte Carlo method; surface analysis; Auger electron spectroscopy

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BIOGRAPHY

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