Monte Carlo Simulation of Backscattering Coefficients for Three Solids

H. I. Imtiaz[1], M. S. S. Khan[2], S. F. Mao[3*], Y. B. Zou[4] and Z. J. Ding[1*]

[1]Department of Physics, University of Science and Technology of China, Hefei, Anhui 230026, China

[2]Key Laboratory of Materials Physics, Institute of Solid State Physics, Chinese Academy of Sciences, Hefei, Anhui 230031, China

[3]Department of Nuclear Science and Engineering, University of Science and Technology of China, Hefei, Anhui 230026, China

[4]School of Physics & Electronic Engineering, Xinjiang Normal University, Urumqi, Xinjiang 830054, China

We have conducted a comprehensive investigation on the electron backscattering coefficients of three elemental and intermediate atomic number solids, namely Cr, Co, and Pd, across a range of primary electron energies of 0.1-100 keV. Our study utilized an up-to-date Monte Carlo simulation model, incorporating a relativistic dielectric functional approach for calculating the electron inelastic cross section [1,2]. In this process, we considered multiple datasets of optical energy loss function (ELF) to account for the influence of different ELF choices on the calculated backscattering coefficients. We observed a significant impact of the chosen ELF datasets on the backscattering coefficients, with the influence following the f- and ps-sum rules and the resulting energy dependence of the electron inelastic mean free path.

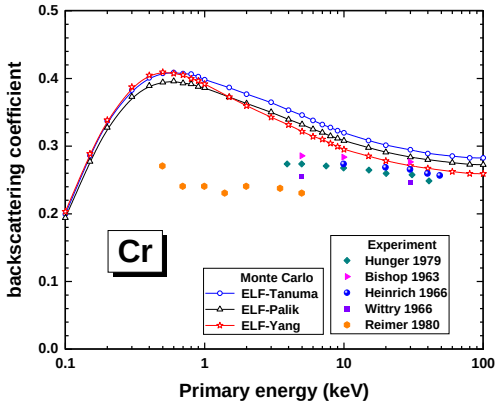

Figure 1. Calculated backscattering coefficient by using three ELF datasets.

To ensure a meaningful comparison with experimental data, we have carefully examined both theoretical uncertainties due to the elastic cross section model and the experimental systematic errors associated with contaminated surfaces. Our analysis revealed that the theoretical uncertainty arising from the elastic cross section model was negligible, as we employed a wide range of 192 scattering potentials to calculate Mott's electron elastic cross section.

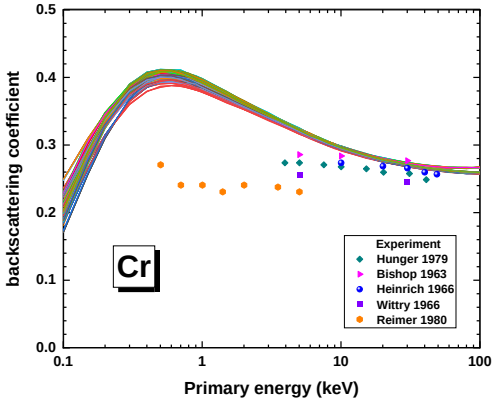

Figure 2. Calculated backscattering coefficient by using 192 elastic scattering models.

Conversely, by simulating contaminated surfaces with the addition of several carbonaceous atomic layers, we successfully accounted for the uncertainty involved in the experimental data. Based on our findings, we emphasize the

*Corresponding Author: sfmao@ustc.edu.cn

*Corresponding Author: zjding@ustc.edu.cn

importance of obtaining accurate backscattering coefficient data from either fully cleaned surfaces or modern Monte Carlo simulations incorporating reliable optical constants data. Furthermore, we express optimism regarding the construction of a reliable theoretical database for electron backscattering coefficients of clean surfaces in elemental solids [3]. This optimism arises from recent advancements in the precise measurement of optical constants through techniques such as reflection electron energy loss spectroscopy. In summary, our study provides valuable insights into the factors influencing electron backscattering coefficients, highlighting the significance of accurate data acquisition and theoretical modeling for future research in this field.

Keywords: Monte Carlo simulation; backscattering coefficient; chromium; cobalt; palladium; energy loss function.

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BIOGRAPHY

Hafiza iman Imtiaz is a PhD scholar from University of Science and Technology of China under the supervision of Professor Ding Zejun. Her research area is Monte Carlo simulation of electron-matter interaction.

*Corresponding Author: sfmao@ustc.edu.cn

*Corresponding Author: zjding@ustc.edu.cn