

Summit to: Materials Database Construction

Reexamination of Monte Carlo simulation of electron emission yields

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EXTENDED ABSTRACT: Electron emission yields, including backscattering coefficient and secondary electron yield, had been an interesting topic for a Monte Carlo simulation long time ago since 1960s. It was widely accepted that a good Monte Carlo modeling should produce calculation results of electron emission yields, at least for backscattering coefficients, in a reasonable agreement with experimental measured data to validate the established Monte Carlo physical model. However, the accumulation of experimental data measured over decades by different research groups has presented a challenge to this belief. This is because a large scattered distribution of data values, particularly for secondary electron yields, has been observed in the database. The cause of the difference is often attributed to the sample condition, e.g. the vacuum and surface cleaning process, in literatures. Therefore, reliable experimental database for clean and smooth surfaces is still lacking. On the other hand, in recent years researchers have made a big progress on the theoretical modeling of electron inelastic scattering with a dielectric function formulation; full electron energy spectrum and the low-loss electron energy loss spectrum can be simulated in a perfect agreement with the measured spectrum. Therefore, there is no reason why the simulated yields which are the area of the energy spectrum should not be the true representation of the yield values of ideal surfaces. We have found that the carbon contamination in several atomic layers can explain well the difference on backscattering coefficient between the simulation and experiment [1,2]. Therefore, we propose to establish a theoretical database of electron emission yields from Monte Carlo simulations for ideal samples which are free of surface contamination and surface roughness. Our latest comprehensive Monte Carlo simulations of electron emission yields for silicon by including all the potential theoretical uncertainty factors have indicated that the combined theoretical uncertainty is very limited. Theoretical calculation of reliable electron emission yields is thus practical and, in fact, on the way.

Keywords: Monte Carlo; backscattering coefficient; secondary electron yield

REFERENCES

- [1] A. Hussain, L. H. Yang, S. F. Mao, B. Da, K. Tókési and Z.J. Ding, *Nucl. Mater. Energy* **26** (2021) 100862.
- [2] L. H. Yang, A. Hussain, S. F. Mao, B. Da, K. Tókési and Z. J. Ding, *J. Nucl. Mater.* **553** (2021) 153042.

BIOGRAPHY



Ding Zejun completed his PhD at the Department of Physics, School of Engineering, Osaka University, Japan in 1990 and four years later performed his JSPS postdoctoral studies at the same laboratory. He is now the director of Laboratory of Microstructure of Solids, Department of Physics, University of Science and Technology of China. He has published over 300 research papers in peer reviewed journals.