A Theoretical Characterization Method for Non-spherical Core-Shell Nanoparticles by XPS

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EXTENDED ABSTRACT: Core-shell nanoparticles (NPs) are active areas of research for their unique properties and wide applications. By changing the elemental composition in core and shell, a series of core-shell NPs with specific functions can be obtained, where the sizes of the core and shell also have influence on the properties. X-ray photoelectron spectroscopy (XPS) is useful in this context as a means of quantitatively analyzing such NPs. The empirical formula proposed by Shard [1] for calculating the shell thickness of the spherical core-shell NPs has been verified by Powell et al. [2-3] through a simulation of XPS with Simulation of Electron Spectra for Surface Analysis (SESSA) software. However, real core-shell NPs are not necessarily ideal spheres; such NPs can have rich shapes and uneven thicknesses. This work aims to extend the Shard formula to non-ideal core-shell NPs. We have used Monte Carlo simulation method to study the XPS signal variation with the shell thickness for several modeled non-spherical shapes of core-shell NPs including some complex geometric structures that are numerically constructed with finite-element triangular meshes. We defined the equivalent radius and equivalent thickness to characterize the average size of the nanoparticles for the use of the Shard formula. We have thus derived an extended Shard formula for the specific core-shell NPs, with which the relative error between the predicted shell thickness and the real thickness can be reduced to less than 10%.

Keywords： Core-shell NPs; XPS; Shard formula; Monte Carlo method

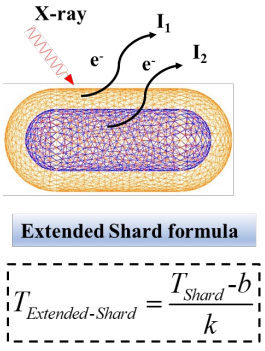

Figure 1. Schematic diagram of non-spherical core-shell NPs and Extended Shard formula.

REFERENCES

[1] A. G. Shard, *J. Phys. Chem. C* **116(31)**, (2012) 16806-16813

[2] C. J. Powell, W. S. M. Werner, A. G. Shard and D. G. Castner, *J. Phys. Chem. C* **120(39)**, (2016) 22730-22738

[3] C. J. Powell, W. S. M. Werner, H. Kalbe, A. G. Shard and D. G. Castner, *J. Phys. Chem. C* **122(7)**, (2018) 4073-4082

BIOGRAPHY

Jiamin Gong has achieved her Bachelor degree at NENU in 2017 and now she is a PH.D. student in the Department of Physics at USTC. Her research interests include surface analysis and Monte Carlo simulation of REELS, AES and XPS spectra.

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