Monte Carlo Study on Secondary Electron Yield of Carbon Nanotube

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Carbon nanotubes (CNTs) are unique carbon nanomaterials with lots of applications in electronics and nanotechnology. Understanding the secondary electron yield (SEY) of CNTs is crucial for characterization of their properties via scanning electron microscopy. Experimental studies have demonstrated that SEY of CNTs depends on several factors, including their diameter, length, number of walls and chirality. In this study we present an investigation into the SEY of CNTs by using a newly developed anisotropic Monte Carlo method combined with the first-principles calculation of electronic excitation in CNTs. This new anisotropic Monte Carlo method provides a universal computational approach towards modelling of anisotropic electron scattering and electronic excitation in anisotropic materials including crystal as well as CNTs. By considering the directional dependence of electron inelastic scattering, the new model captures the intricate behavior of electrons within CNTs more accurately than the traditional isotropic scattering models.

The optical properties together with the conductivity of multi-walled carbon nanotubes (MWCNTs) vary with their wall thickness. Different wall thicknesses of MWCNTs exhibit distinct optical behaviors and, hence, the related electronic excitation. By using the first-principles calculation based on density functional theory (DFT) the energy loss function (ELF) of single-walled carbon nanotube (SWCNT) was firstly obtained in the photon energy range of 0.1-30 eV. Furthermore, from the calculated density of SWCNT one can use the ELF of graphite to derive the ELF of carbon nanotube in the high photon energy region, leading to the derivation of the full ELF from the low to high energy losses.

We have investigated how the anisotropic characteristics of SWCNT affect the SEY. Low values of SEY of SWCNT were obtained from the Monte Carlo simulation, which reasonably agree with the experimental data [1]. The insights gained from this study not only help the advance of our understanding of electron-CNT interactions but can also offer practical guidance for optimizing CNT-based electron emission devices. The application of anisotropic Monte Carlo methods can also provide a powerful tool for studying CNTs in depth, contributing to the advancement of nanotechnology and electronic devices. Our future research directions include further refinement of simulation model to capture the character of charging effect and to validate it with experimental studies.

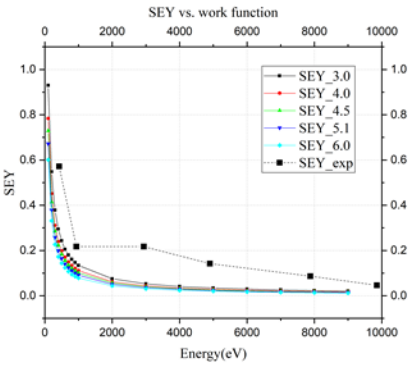

Figure 1. Comparison on the SEY of SWCNT between simulation and experiment.

Keywords: Monte Carlo simulation; carbon nanotubes; secondary electron yield; energy loss function.

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BIOGRAPHY

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