Theoretical Modeling of Secondary Electron Yield Using First-Principles Input: Comparison with Experimental Measurements

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Abstract: *Secondary electron yield of a material is a crucial factor in designing many electronic devices, from electron multipliers to high-power radio frequency devices used in the aerospace industry. In the latter, it is key in mitigating the highly destructive multipactor, where a low value of secondary electron yield is desired. In this work we present results for select elemental metals obtained using a newly developed, state-of-the-art, Monte Carlo code for modeling secondary electron emission with entirely first principle input. The results are compared with the available experimental data.*

Keywords: secondary electron emission; secondary electron yield; multipactor; density functional theory; Monte Carlo modeling

Introduction

Secondary electron emission is an effect in which electrons are emitted from a target due to electron irradiation. It is the working principle of an electron scanning microscope, electron multipliers, and various other electronic devices. Its magnitude, the secondary electron yield (SEY), is also a key property governing multipactor. Multipactor is an effect in which electrons exponentially multiply causing interference and breakdown of vacuum radio frequency (RF) devices, often used in the aerospace industry where they are expensive and difficult to access and replace or repair. The use of low SEY materials in designing RF devices could help suppress multipactor, therefore, finding such materials is highly desired. Experimental measurement of SEY are not only demanding but also require access to well prepared samples, therefore, computational modeling potentially provides a fast and inexpensive alternative, especially for screening many candidate materials.

In this work, we combine first principles density functional theory (DFT) and Monte Carlo (MC) simulations to calculate the SEY of 25 elemental metals using state-of-the-art methods. MAterials Simulation Toolkit for Secondary Electron Emission (MAST-SEY) [1], a newly developed, open-source MC code was used in the modeling, allowing us to employ entirely first principles input.

In the present model, the electrons within the metal can be scattered either elastically or inelastically [2]. Mott's theory [3] is employed to describe the elastic interactions. The inelastic scattering is governed by the differential inverse inelastic mean free path (IMFP):

$$\frac{d^2\lambda_{in}^{-1}}{dqd\omega} = \frac{\hbar}{\pi a_0 E}\mathrm{Im}\left\{\frac{-1}{\varepsilon(q,\omega)}\right\}\frac{1}{q}$$

Where λ_{in}^{-1} is the IMFP, q is the wavevector, $\varepsilon(q,\omega)$ is the energy and wavevector dependent dielectric function, E is the incident energy, and $\hbar$ and a_0 are Planck's constant and Bohr radius, respectively. The integration of the differential inverse IMFP allows to obtain IMFP, for which the wavevector dependence of the dielectric function is needed. For this purpose, the Penn approach [4] is most commonly utilized, however, the recent advancements in time dependent DFT allow for explicit, first-principle calculation of the wavevector dependence of the dielectric function [5]. This approach provides a more accurate description of the momentum transfer, and therefore, the IMFPs as well. More details on the DFT calculations can be found in [6]. The new MAST-SEY code is capable of using the single pole Penn approximation as well as utilizing TDDFT results.

Results and Discussion

25 metallic systems (elemental metals) have been investigated and compared with the available experimental data. Literature study of experimental measurements reveals a large discrepancy in reported values, with the spread in values often as high as 200%. An example of a few experimental datasets alongside a modeled curve can be seen in Fig. 1.

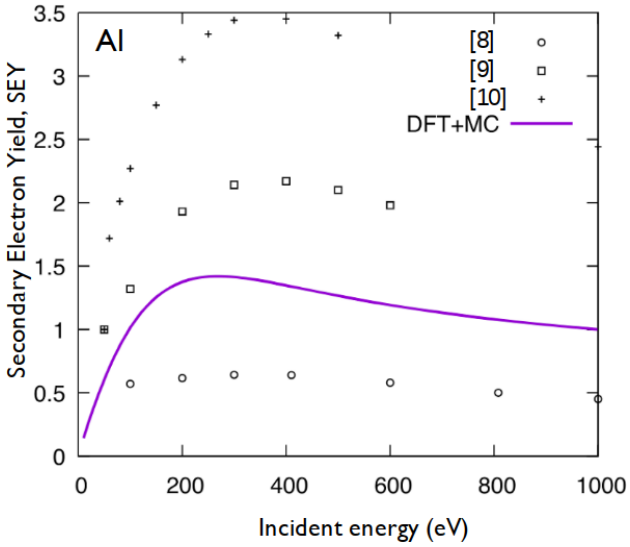

Figure 1. Comparison of the results of the modeling with available experimental data.

The main cause of the experimental discrepancies can be connected with the difficulties in controlling the surface of the measured sample and different surface preparation protocols used. The differences in equipment and measuring techniques, especially considering the timespan of the reports, may also be a contributing factor. At the present date, no comprehensive and consistent experimental study has been performed, and the most accurate data seem to be the modeling assisted examination of the experimental data performed by Lin and Joy [7]. The calculations performed here use consistent methods and assume a perfect surface for each studied system. The entirely theoretically obtained SEY, after comparison with the database does not reveal a clear correlation between theory and experiment. This result suggests a deeper issue with the experimental measurements or significant missing physics or numerical issues in the simulation. Considering the methodologically advanced modeling and the well known problems with the control of the consistency of measurements, it seems that a consistent study of a range of materials is needed in order to progress in the search of low SEY materials to aid in verification of the modeling and assessing its predictive power and potential limitations. Such studies, combining state-of-the-art theory and experiment, are a part of an ongoing research within our multi-university MURI collaboration.

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