Density Functional Theory Calculations for the Simulation of Secondary Electron Yield

Ivana Matanovic[1], Maciej P. Polak[2], Ryan S. Johnson[3], Raul E. Gutierrez[3], Dane Morgan[2], and Edl Schamiloglu[3]

[1]Dept. of Chemical and Biological Engineering, University of New Mexico Albuquerque, NM 87131, USA

[2]Materials Science and Engineering University of Wisconsin 1415 Engineering Dr., Madison, WI 53706, USA

[3]Dept. of Electrical and Computer Engineering University of New Mexico Albuquerque, NM 87131, USA

Abstract: *Suppressing the harmful multipactor effect by, for instance, reducing secondary electron yield (SEY) is crucial in the design of RF space technologies. Therefore, improving fundamental understanding of how structural and electronic features of materials affect the SEY is necessary. In this benchmark work, we use density functional theory calculated properties to simulate, via Monte Carlo method, the SEY of simple metals copper and silver. As in these simulations the dielectric property i.e. the energy and momentum dependent energy loss function plays a major role, we focus our study on the computational procedures necessary to obtain reliable first principles data.*

Keywords: multipactor, secondary electron yield, momentum dependent energy loss function, density functional theory, Monte Carlo simulations of secondary electron yield, MAST-SEY code

Introduction

Suppressing the harmful multipactor behavior, an avalanche-like discharge of electrons occurring in devices operating under high vacuum and high-power RF electromagnetic fields, is crucial in the design of space technologies. The use of materials with low secondary electron yield (SEY) helps mitigate multipactor breakdown and decreases the performance deterioration in various RF electronic devices. This work tests the applicability of first principles approaches to provide reliable data for Monte Carlo (MC) simulations, initially for simple benchmark metals. Moreover, studying how different density functional theory (DFT)-calculated properties affect SEY can provide a fundamental insight into the key electronic or structural features of the materials that can reduce SEY and mitigate the multipactor effect. Towards realizing this goal, we first perform electronic structure calculations based on DFT to calculate energy and momentum dependent energy loss function as well as the density of states and Fermi energy of Cu and Ag. These are then used as inputs for the MC simulations to predict the SEY of Ag and Cu.

Results and Discussion

DFT calculations were performed using all-electron full-potential linearized augmented plane-wave method as implemented in *exciting* code [1]. Ground-state electron densities and Kohn-Sham eigenvalues and eigenfunctions have been obtained using PBE exchange-correlation functional. The energy loss functions were calculated within the linear-response formalism of time-dependent DFT *via* random-phase approximation kernel using off symmetry 30x30x30 *k*-point mesh.

Fig. 1 shows the frequency dependent energy loss functions of Cu and Ag. The origin of the main peaks in the loss function of Cu and Ag has been analyzed in detail previously [2,3]. In short, peaks below 10 eV have been classified as plasmon resonances while the eminent features in the loss function for energies from 10 to ~60 eV were attributed to the interband transitions from *d* states to unoccupied states above the Fermi level. At higher energies semi-core and core excitations, such as excitations from lower-lying *s*- and *p*- levels, start to contribute. Except for the low plasmon peak of Ag at ~3.8 eV, comparison with the experimental curves [3,4] shows that all-electron electronic structure calculations used in this work provide a good description of the dielectric properties of Ag and Cu. Furthermore, in agreement with previous studies [2,3] our analysis show that the local field effects are essential for the correct description of the energy loss at energies > 40 eV in Ag, while they have a much smaller effect on energy loss in Cu.

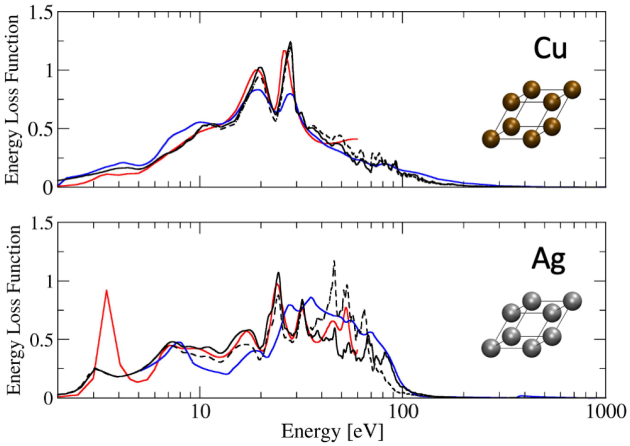

Figure 1. Energy loss function of Cu and Ag (black) for small momentum transfers (0.002/Bohr) in comparison to experimental data from Ref. [3] (red) and Ref. [4] (blue). Black dashed lines indicate energy loss function calculated without local-field effects.

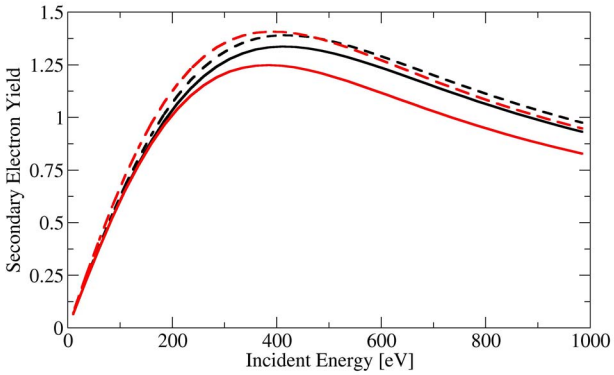

Figure 2. SEY of Cu (black) and Ag (red) obtained by universal curve fitting [5] of MC simulated data. In the MC simulations we used inelastic scattering cross sections obtained with Penn's single-pole approximation [6] applied to DFT calculated energy loss functions from Fig. 1. Dashed lines correspond to SEY curves obtained with the use of DFT energy loss functions without local-field effects.

The SEY of Ag and Cu (Fig. 2) is obtained through MC simulations as implemented in the MAST-SEY MC code [7]. In this approach the inelastic electron scattering is described by inelastic scattering cross sections obtained with the use of the Penn's single-pole approximation [6] applied to DFT calculated energy loss functions from Fig. 1. Work function for Cu and Ag are set to 4.53 and 4.22 [8] in order to match the ones of polycrystalline samples. The MC results show that for Cu SEY maximum of 131% is calculated at an incident energy of 413 eV, while for Ag the SEY maximum is calculated as 122% at an incident energy of 384 eV. The results further show that including local field effects in the calculation of energy loss function has a large effect on SEY of silver and almost negligible effect on SEY of Cu. Excluding local fields in the calculation of energy loss function results in the maximum SEY of 136% at 417 eV and 137% at 392 eV for Cu and Ag, which results in 4% and 12% yield increase, respectively.

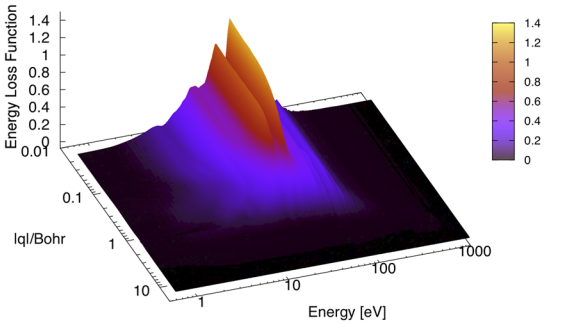

Figure 3. DFT calculated energy loss function of Cu as a function of momentum q in the (100) direction. Local field effects not included.

MC procedure used to obtain SEYs on Fig. 2 approximates q-dependence of energy loss function; therefore, we further use DFT to calculate the energy loss function as a function of momentum transfer in different crystallographic directions. Fig. 3 shows the energy loss function of Cu where momentum transfer is along (100) direction, and varies between 0.0016 and 16/Bohr. The general trend seen in Fig. 3 is that the absolute value of the loss function decays with increasing momentum q. Furthermore, q-dispersion of peaks' position depends on the origin of the peak [3]. While plasmons peaks show quadratic dependence of the peak position, the peaks above 10 eV show very little change in the position of their maxima as q increases. Dependencies such as the one on Fig. 3 allow for the calculation of the inelastic electron scattering and SEY directly from *ab initio* calculated q-dependent energy loss function, which is a part of an on-going effort.

Conclusions and Future Work

All-electron calculations based on time-dependent DFT and with local field effects were able to achieve a reliable description of dielectric properties of Cu and Ag. Moreover, they allow for the computation of q-dependent energy loss functions, which can be used for the prediction of SEYs based entirely on the first principles-calculated properties of the material. Future work includes detailed examination of surface effects and further benchmarking of the developed DFT-MC approach to predict SEYs of more complex materials such as alloys.

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