Monte Carlo Simulation of Secondary Electron Emission from Metals and Insulators
(co-directed with R.J. Friauf)

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Models are proposed to describe the various scattering processes that are involved in secondary electron emission (SEE) from metals and insulators, with the major emphasis on insulators. In insulators we use the dielectric theory to calculate the cross section of scattering resulting from the interaction of the incident electron traveling through the solid with and the excitation of electrons in the topmost valence band, which are the most important electrons for secondary electron production. Partial wave analysis is used to calculate the cross section for elastic scattering. A formulation for free atom ionization is used to treat the ionization of inner shell electrons. These scattering cross sections are used in a Monte Carlo simulation to determine yield, energy distribution and angular distribution of the secondary electrons.

For the dielectric theory we have calculated a wave number and frequency dependent dielectric function $\epsilon(q, \omega)$ using the random–phase approximation for a model insulator originally proposed by Fry (1969). In our calculations, however, we assumed an fcc crystal structure with no further simplifications. Furthermore, we included both the first and second conduction bands. For the real part of the dielectric function we performed a numerical principal value integration over the first and second Brillouin zones. For the imaginary part we performed a numerical integration involving the δ function that results from the conservation of energy. The validity of our numerical integration method was checked by applying the Kramers–Kronig transform to the results.

Experimental results suggest that band gap E_g and electron affinity χ are the most important quantities affecting the SEE yield of insulators. Therefore, by adjusting the free parameters of the model insulator we make the model to represent a material from each of the group of wide band gap (solid Ar with $E_g = 13.3$ eV and $\chi = 0$), medium band gap (KCl with $E_g = 8.5$ eV and $\chi = 0$), and small band gap (Si with $E_g = 1.12$ eV and $\chi = 4.05$ eV) insulators. The most striking feature of our Monte Carlo simulatio results is that the maximum yield turns out to be 8 to 10 for wide and medium band gap insulators, about 1 to 2 for small band gap insulators, and about 0.7 for metals, which agrees very well with the trend observed experimentally. Among the other studies discussed in this work are: the effect of E_g by itself on the SEE yield when χ is constant, the effect of χ by itself when E_g is kept constant, the energy and angular distribution of the secondary electrons for normal angle of incidence.