Summary Abstract: Dependence of inelastic electron mean free paths on electron energy and material

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The inelastic mean free paths (IMFP's) of low-energy electrons in solids are important for defining the surface sensitivities of electron spectroscopies for surface characterization. We have developed a new general formula for predicting IMFP's over the electron energy range 200–2000 eV.[1] This formula allows convenient determination of the IMFP dependence on electron energy for a given material and the material dependence for a given energy.

We have made separate IMFP calculations for 27 elements (C, Mg, Al, Si, Ti, V, Cr, Fe, Ni, Cu, Y, Zr, Nb, Mo, Ru, Rh, Pd, Ag, Hf, Ta, W, Re, Os, Ir, Pt, Au, and Bi) and 4 compounds (LiF, Al_2O_3, SiO_2, and ZnS) using an algorithm due to Penn.[2] IMFP's are calculated using experimental optical data to describe the dependence of the inelastic scattering probability on energy loss and the Lindhard dielectric function to describe the dependence of the scattering probability on momentum transfer. Details of the calculations are given elsewhere.[1,3]

For each material, IMFP calculations were made for electron energies between 100 and 2000 eV. For energies between 200 and 2000 eV, the IMFP's could be satisfactorily fitted to the Bethe equation for inelastic electron scattering:

$$\lambda_i = E/[E_p^2\,\beta \ln(\gamma E)]\ \text{Å}, \tag{1}$$

where λ_i is the IMFP, E the electron energy (in eV), and

$$E_p = 28.8(\rho N_v/A)^{1/2}\ \text{eV}. \tag{2}$$

N_v is the total number of valence electrons per atom or molecule, the density ρ has been expressed in g cm^{-3}, and A is the atomic or molecular weight. For a metal such as copper, N_v is computed from the number of 4s and 3d electrons, in this case 11. Values of the two parameters β and γ in Eq. (1) have been determined from fits of the calculated IMFP values for each material to the Bethe equation. We have found that these parameters could be related empirically to simple material constants. Least scatter was found with the following equations:

$$\beta = -2.52\times10^{-2} + 1.05/(E_p^2 + E_g^2)^{1/2} + 8.10\times10^{-4}\rho \tag{3}$$

and

$$\gamma = 0.151\rho^{-0.49}, \tag{4}$$

where E_g is the band-gap energy (in eV) for nonconductors. The average rms difference between the individual IMFP calculated values and the results of Eqs. (1)–(4) for the 31 materials was about 12%, the largest differences being for C (32%), ZnS (31%), Ir (27%), SiO_2 (26%), Re (21%), Si (19%), Pd (18%), Nb (17%), Bi (16%), Ta (16%), and Ni (16%). These differences were not considered excessive on account of uncertainties of the optical data, the empirical basis of Eqs. (3) and (4), and the small number of nonconductors in the analysis.

The solid line in Fig. 1 shows the present IMFP results for silicon and the curve labeled TPP indicates IMFP's from our proposed general formula [Eqs. (1)–(4)]. The curve designated SLJL gives IMFP's calculated from a formula due to Szajman *et al.*[4]

While the IMFP is usually obtained from theory and some types of experiments, the quantity often measured is the at-

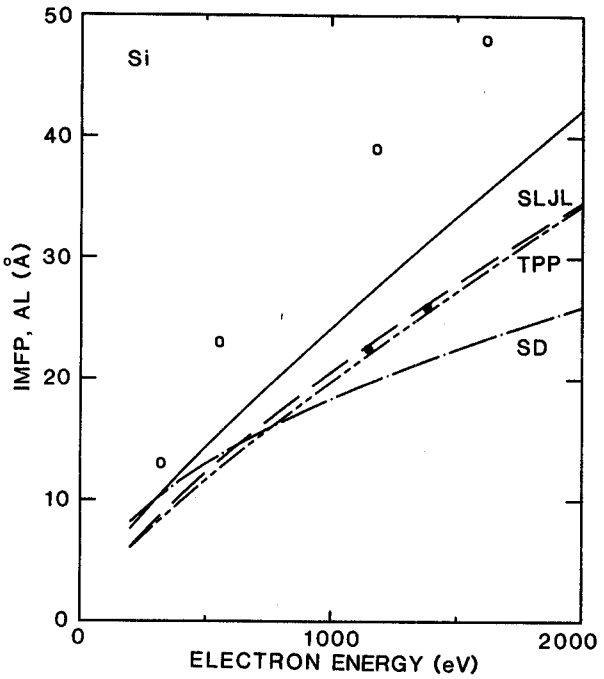

FIG. 1. Comparison of IMFP and AL results for Si (see text for details).

tenuation length (AL); the AL is obtained from overlayer–film experiments and with use of a model in which the effects of elastic electron scattering are ignored.[5] It has been estimated that the IMFP may exceed the AL by about 15%, the difference being greatest for high atomic numbers and low electron energies.[6] Figure 1 shows the early AL results of Klasson *et al.*[7] (open circles). The solid circles show the AL results of more recent experiments.[8] The curve designated SD gives AL's calculated from the empirical formula of Seah and Dench.[9]

Since errors in AL measurements are often considerable[5] and there are approximations in IMFP calculations,[2] it is difficult to assess reliability from comparisons of the type shown in Fig. 1. Nevertheless, this and other comparisons[1] indicate that Eqs. (1)–(4) provide a convenient means for determining the IMFP dependence on electron energy for a particular material in the range 200–2000 eV and the IMFP dependence on matrix or material for a given energy. The new formula should also be a useful but more approximate guide for estimating AL's.

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