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Electron inelastic mean free paths in compounds

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We have calculated inelastic mean free paths (IMFPs) for 45 compounds for electron energies over the 50 eV to 200 keV range with the full Penn algorithm from the energy-loss functions of the compounds. Our calculated IMFPs could be fitted to a modified form of the relativistic Bethe equation for inelastic scattering in matter for energies from 50 eV to 200 keV. The average root-mean-square deviation in these fits was 0.60 %. The IMFPs were also compared with a relativistic version of our predictive Tanuma-Powell-Penn (TPP-2M) equation.

1. Introduction

Information on the inelastic scattering of electrons in solids is important for various applications ranging from radiation physics and radiation transport to thin-film analysis in the transmission electron microscope (TEM) and surface analysis by Auger-electron spectroscopy and X-ray photoelectron spectroscopy. A key parameter in these applications is the electron inelastic mean free path (IMFP).

Therefore, we previously calculated IMFPs for many solid materials over a wide energy range.[1-8] Initially, we reported IMFPs for 50 eV to 2,000 eV electrons for 27 elemental solids, 15 inorganic compounds, and 14 organic compounds. We analyzed these calculated IMFPs with the Bethe equation for inelastic scattering of electrons in matter to develop an IMFP predictive formula (designated TPP-2M).[4] The TPP-2M equation could be used to estimate IMFPs in other materials, again for energies between 50 eV and 2,000 eV, the energy range of interest for many AES and XPS experiments.

Since there is a need for IMFPs in transmission electron microscopy (TEM), we also calculated IMFPs in 41 elemental solids for energies up to 200 keV with a relativistic version of the full Penn Algorithm (FPA).[7] In addition, we developed a relativistic version of the TPP-2M equation that provides reasonable IMFP estimates for energies between 50 eV and 200 keV. The root-mean-square (RMS) deviation between the estimated IMFPs from the TPP-2M equation and the directly calculated values was 11.9 % for the group of 41 elemental solids.[7] This RMS deviation was similar to that found (10.2 %) in a similar comparison for our original group of 27 elemental solids for the 50 eV to 2 keV energy range.[4]

In this presentation, we will report calculations of IMFPs with the relativistic FPA using the Boutboul approach [9] for 45 compounds (AgBr, AgCl, AgI, Al_2O_3, AlAs, AlN, AlSb, cubic BN (*c*-BN), hexagonal BN (*h*-BN), CdS, CdSe, CdTe, GaAs, GaN, GaP, GaSb, GaSe, H_2O, InAs, InP, InSb, KBr, KCl, LiF, MgF_2, MgO, NaCl, $NbC_{0.712}$, $NbC_{0.844}$, $NbC_{0.93}$, PbS, PbSe, PbTe, Si_3N_4, SiC, SiO_2, SnTe, $TiC_{0.7}$, $TiC_{0.95}$, $VC_{0.76}$, $VC_{0.86}$, $Y_3Al_5O_{12}$, ZnS, ZnSe, and ZnTe) for energies between 50 eV and 200 keV. The IMFPs for most of these compounds (exceptions H_2O, LiF, and Si_3N_4) have already been published [8].

2. IMFP Calculations with the Relativistic Full Penn Algorithm

The IMFPs were calculated with the relativistic FPA that includes the bandgap effect with the Boutboul approach for semiconductors and insulators at equal energy intervals on a logarithmic scale corresponding to increments of 10 % from 10 eV to 1 MeV. We will present IMFPs for energies between 10 eV and 50 eV

and between 200 keV and 1 MeV in Figures but these results are shown only to illustrate trends. The IMFP, λ, at electron energy T ($>E_g + E_v$), which is measured from the bottom of the valence band for semiconductors and insulators, can be expressed as :

$$\lambda(T)^{-1} = \frac{\left(1 + T'/c^2\right)^2}{1 + T'/\left(2c^2\right)} \frac{1}{\pi T'} \iint_D \frac{1}{q} \mathrm{Im}\left[\frac{-1}{\varepsilon(\omega, q)}\right] dq d\omega$$

where $T' = T - E_g$ and E_g is the bandgap energy. The integration domain D is determined from the maximum and minimum energy losses and the largest and smallest kinematically-allowed momentum transfers for a given energy T and ω:

$D = \{(\omega, q): E_g \le \omega \le (T' - E_v), q_- \le q \le q_+\}$,

where Ev is the width of the valence band for semiconductors and insulators, and

$q_\pm = \sqrt{T'(2 + T'/c^2)} \pm \sqrt{(T' - \omega)[2 + (T' - \omega)/c^2]}$.

3. Results and discussion

3.1 Effect of the bandgap energy on the calculated IMFPs

The value of the bandgap energy E_g is an important parameter in the calculations of IMFPs for nonconductors, as shown in the above equations. We therefore investigated the influence of including the E_g value on the calculated IMFPs for several compounds including Si_3N_4 and LiF. The inclusion of the bandgap energy in the IMFP calculation generally leads to IMFP increases for E < 100 eV. This increase is due to the decrease in the ω (or energy) integral domain D. The lower limit of the ω integral, ΔE_{min}, is set equal to the bandgap energy for nonconductors. This limit corresponds to the minimum excitation energy for electrons in the material. The maximum excitation energy corresponds to the upper limit of the ω integral, ΔE_{max}. This upper limit ensures that an incident electron will always have sufficient energy to remain in the conduction band. The upper limit is then given by $\Delta E_{max} = T - E_v - E_g$. On the other hand, ΔE_{min} and ΔE_{max} for conductors are given by 0 and T - E_f, respectively, where E_f is the Fermi energy.

For $T - E_v$ - $E_g \ge 100$ eV, we found that the IMFPs from the FPA-Boutboul approach are larger than the IMFPs from the FPA with E_g assumed to be zero by less than 1.3%. For lower energies, the IMFP differences become larger due to the decrease in the ω integral domain, reaching 30 % and 7.3 % at 49.4 eV for LiF and Si_3N_4, respectively.

We conclude that the effect of the bandgap energy on IMFPs calculations with the FPA is generally small (< 1.5 %) for energies over 100 eV even for materials that have large bandgap energies such as SiO_2.

3.2 Comparison of IMFPs with measured IMFPs

We also compared our calculated IMFPs for Al_2O_3, AlAs, *h*-BN, GaAs, InP, MgO, and SiO_2 with 71 measured IMFPs for these compounds. These IMFP measurements have most often been made by elastic-peak electron spectroscopy for energies between 100 eV and 5 keV and by TEM at energies of 100 keV, 200 keV or 300 keV, while some measurements were made for GaAs at energies between 24 eV and 140 eV by photoelectron spectroscopy. We found generally satisfactory agreement between the calculated and measured IMFPs with an average RMS deviation of 23.5 % although some TEM IMFPs for AlAs and GaAs were smaller than our values by 48 % and 45 %, respectively. If these two measurements are disregarded, the average RMS difference between our calculated IMFPs and the 69 other measured IMFPs was 18.7 %. This average RMS difference is comparable to the average RMS difference between calculated and measured IMFPs of 13.6 % for 11 elemental solids at 100 keV and for 32 elemental solids at 200 keV.[7]

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