Energy dependence of the mean free path of excess hot electrons in solid xenon in the elastic scattering region

B. Plenkiewicz, P. Plenkiewicz, and J.-P. Jay-Gerin*
Groupe du Conseil de Recherches Médicales du Canada en Sciences des Radiations et Département de Médecine Nucléaire et de Radiobiologie, Faculté de Médecine, Université de Sherbrooke, Sherbrooke, Québec, Canada J1H 5N4
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It has been found recently from the analysis of low-energy electron-transmission experiments that the scattering mean free path λ of excess hot electrons in solid xenon films oscillates with energy. We show in this paper that in these experiments λ is predominantly controlled by the combined effect of both acoustical-phonon scattering and scattering by neutral point defects, and that its energy dependence is entirely caused by the changes in electron effective mass with energy.

So far, little is known regarding the magnitude and the energy dependence of the scattering mean free path (MFP) of excess electrons of energies of a few electron-volts in semiconductors and insulators. A knowledge of the electron scattering MFP is important for the interpretation of photoemission, low-energy electron diffraction, and electron-transport data, and is also needed to obtain quantitative and energy-dependent results about electron interactions in dielectric solids. Up to electron kinetic energies of about a few tenths of an electron-volt, information about electron-transport properties in rare-gas solids is available from drift-mobility measurements.[1] At higher energies, however, hot-electron transport has not received much attention until recently. Bader *et al.*[2] were the first authors who tried to determine the electron MFP and its energy dependence in solid xenon from the analysis of low-energy electron-transmission experiments. They used a two-stream approximation based on a classical description of the electron-transport problem and previously developed for studying the motion of electrons in gases. Recently, Plenkiewicz *et al.*[3] proposed a theoretical model, based on the quantum theory of solids, to analyze the experimental electron-transmission results in solid xenon in a much simpler way. This model allowed them to obtain, among other things, the magnitude and the energy dependence of the electron MFP in the elastic scattering region. In this energy region, the electron MFP was found to oscillate as a function of energy. In an attempt to explain the origin of such a behavior, we have performed an independent calculation of the scattering MFP of excess hot electrons in rare-gas solids, taking the case of solid xenon as an example. In this paper, we present the results of this calculation.

Electrons injected into the solid propagate in Bloch states with an effective mass m^* which is a function of the electron energy; a result of the fact that electrons with different energies occupy different bands. In order to evaluate the energy dependence of m^* in solid xenon, we used the formula[4]

$$m^{*-1}(E) \propto \left[\frac{d^2E}{dk^2}\right], \tag{1}$$

where $E(k)$ is the band energy at wave vector k, in combination with the orthogonalized-plane-wave tight-binding electron band-structure results obtained by Reilly.[5] In the calculation of $m^*(E)$, the E-versus-k dispersion curves for the conduction bands were first represented in terms of appropriate polynomial approximations, and then the electron effective masses were computed analytically using Eq. (1). If more than one conduction band were present at the same energy, we used an averaged effective mass whose inverse was simply defined as[6]

$$\frac{1}{m^*(E)} = \frac{1}{n}\sum_{i=1}^{n}\left[\frac{1}{m_i(E)}\right], \tag{2}$$

where n is the number of conduction bands and $m_i(E)$ are the electron masses corresponding to each of these bands. Figure 1 shows the energy dependence of $(m^*/m_0)^{-1}$ (where m_0 is the free-electron mass) in solid xenon which resulted from this calculation. It should be noted that the electron masses reported in Fig. 1 were normalized by using the value $m^*(0)=0.51m_0$ calculated by Reilly[5] for the effective mass at the conduction-band minimum (chosen here as the zero energy).

Since optical lattice modes of vibration do not occur in the rare-gas solids, the electron MFP in a sufficiently pure and perfect specimen and in the elastic scattering region should be determined solely by acoustic-mode scattering. To calculate the electron MFP λ_{ph} in solid xenon resulting from the scattering of electrons by acoustical phonons, we applied the results of a theory developed by Conwell and Brown[7] for lattice mobility of hot electrons in germanium. According to these authors, the electron relaxation time for acoustical mode scattering is given by[7]

$$\frac{1}{\tau_{ph}} = \frac{\sqrt{2}v_s}{l}\left[\frac{k_BT}{m^*v_s^2}\right]^{5/2}\left[\frac{k_BT}{E}\right]^{3/2} \times \int_0^{(2m^*v_s^2E)^{1/2}/k_BT} du\, u^4 \coth u\ , \tag{3}$$

where

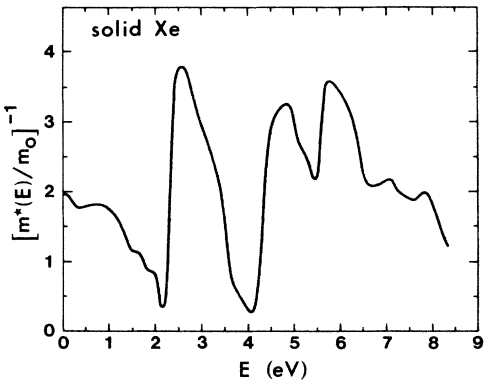

FIG. 1. Energy dependence of $(m^*/m_0)^{-1}$ for solid xenon in the elastic scattering region. The energy of the bottom of the conduction band is chosen as the zero energy.

$$l=\frac{\pi\hbar^4 c}{m^{*2}D^2k_BT}\ , \tag{4}$$

v_s is the sound velocity in the solid, D is the deformation-potential electron-phonon coupling constant, c is an average elastic constant, k_B is Boltzmann's constant, and T is the absolute temperature. It is of interest to write down here the limiting forms of Eq. (3) for small and large values of the ratio (E/k_BT). In the limit $(E/k_BT)\ll 1$, u is small and Eq. (3) reduces to the familiar result $1/\tau_{\rm ph}=(2E/m^*)^{1/2}/l$, or v/l, where v is the electron velocity. Thus, the electron-phonon scattering MPF $\lambda_{\rm ph}$ in this case is simply equal to l. Since $m^*\approx m^*(0)$ has a constant value in the limit of small E, $\lambda_{\rm ph}$ is independent of the electron energy in this region. In the other limit, where $(E/k_BT)\gg 1$, the integral in Eq. (3) is well approximated by setting $\coth u=1$. Then,

$$\frac{1}{\tau_{\rm ph}}\approx\frac{8}{5}\frac{v_s}{l}\frac{E}{k_BT}\ . \tag{5}$$

Thus, at high enough E, $\lambda_{\rm ph}$, defined as $\lambda_{\rm ph}=v\tau_{\rm ph}$, depends on the electron energy through the factor $lv/E\propto 1/(E^{1/2}m^{*5/2})$. If m^* were a constant, $\lambda_{\rm ph}$ would decrease monotonically with E as $1/\sqrt{E}$. Such a result is not true in solid xenon where m^* is a complicated function of E in the limit of high E (see Fig. 1); $\lambda_{\rm ph}$ in this case directly reflects the dependence of m^* on E. Regarding the magnitude of $\lambda_{\rm ph}(E)$, our calculated values in solid xenon at 45 K in the elastic scattering region $E<8.4$ eV (Ref. 8) differ significantly from those of the electron MFP directly obtained from the analysis of low-energy electron-transmission experiments.[2,3] In particular, our calculation predicts much larger values for $\lambda_{\rm ph}(E)$. This result teaches us that, in the adsorbed solid Xe films investigated in those experiments, the electron MFP is not controlled solely by acoustical-phonon scattering, and that another scattering mechanism must be invoked if we want to reproduce quantitatively the electron MFP values obtained from such experiments. Of all possible types of scattering which can be called upon in this problem, the scattering of the incident electrons by neutral point defects created during the growth of the experimental films is thought to be the most likely.[9] Other mechanisms, such as electron-impurity scattering and scattering at crystallite boundaries, also exist but should in fact be very improbable if we judge (i) from the very small amounts (<25 ppm) of impurities present in the films,[2] and (ii) from the films' polycrystalline structure which has been shown to consist of ensembles of grains of relatively large dimensions.[10] Using the results of Erginsoy's work,[11] the scattering of electrons by neutral point defects can be described by means of a relaxation time τ_d given by the equation (in cgs units)

$$\frac{1}{\tau_d}=\frac{20\epsilon\hbar^3}{m^{*2}e^2}N_d\ , \tag{6}$$

where ϵ is the dielectric constant of the medium, e is the electronic charge, $\hbar$ is Planck's constant divided by 2π, and N_d is the concentration (per cm^3) of neutral point defects. As we can see, the neutral-point-defect-limited motion of electrons is a function of the electron energy through the dependence of m^* on E. In the problem at hand, we treated N_d as an adjustable parameter to be determined by requiring that the magnitude of the total electron MFP λ, calculated from $\lambda=v\tau$, where $v=(2E/m^*)^{1/2}$ and $\tau^{-1}=\tau_{\rm ph}^{-1}+\tau_d^{-1}$ [see Eqs. (3) and (6)], be globally similar to that of the electron MFP obtained directly from electron-transmission experiments.[2,3] For the 45-K solid Xe films investigated in these experiments, the value of N_d determined in this way was estimated to be between about 3 and 6×10^{20} cm^{-3}, which corresponds to approximately 2–3 % of defects. The sensitivity of our results to the chosen value of N_d is shown in Fig. 2, which gives the results of our calculations for λ as a function of electron energy $E<8.4$ eV (Ref. 8) for three different values of N_d, namely, 3×10^{20} cm^{-3} (curve a), 6×10^{20} cm^{-3} (curve b), and 10^{21} cm^{-3} (curve c), respectively. The electron scattering MFP obtained from our previous analysis[3] of the electron-transmission experiments in solid Xe films at 45 K is also included in Fig. 2 for the sake of comparison (dashed curve). Physical parameters used in the calculations were $D=1.4$ eV,[12,13] $v_s=0.804\times10^5$ cm/s,[14] $c=\rho v_s^2=2.41\times10^{10}$ erg/cm^3,[14] where $\rho=3.73$ g/cm^3 is the density of solid xenon at 45 K,[14] and $\epsilon=1.98$.[15] As can be seen from Fig. 2, over the range of energies considered, our calculations agree well with experiment. In fact, all of the peaks observed in the $\lambda(E)$ curve obtained from experiment, and their corresponding energy positions are correctly reproduced by the calculation. The λ-versus-E curves differ only in the relative amplitudes of the different peaks. The reasons which might be invoked to explain these differences are (i) the simplified procedure used in the calculation of the electron effective mass, (ii) the ill-defined value of the deformation-potential electron-phonon coupling constant D in solid xenon,[12,13] (iii) the rather approximative character of Erginsoy's formula for describing the problem of electron scattering by neutral point defects,[11] (iv) the possible contributions due to other scattering mechanisms neglected in the present calculations, such as electron-impurity scattering or scattering at crystallite boundaries, and (v) the uncertainty attached to the $\lambda(E)$ curve obtained directly from experiment.[3] A final remark should

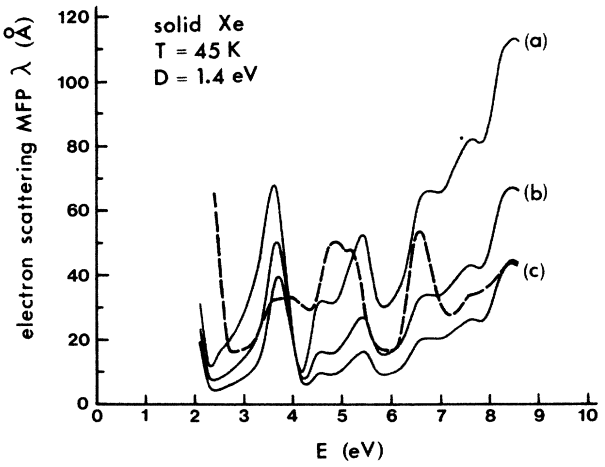

FIG. 2. Plots of the electron scattering MFP λ in solid xenon at a temperature of 45 K as a function of energy in the elastic scattering region. The solid lines are the results of our calculation combining acoustical-phonon scattering and scattering by neutral point defects, and using Eqs. (3) and (6) with $\lambda=v\tau$, where $v=(2E/m^*)^{1/2}$ and $\tau^{-1}=\tau_{\rm ph}^{-1}+\tau_d^{-1}$, for three different values of N_d, namely, 3×10^{20} cm^{-3} (curve *a*), 6×10^{20} cm^{-3} (curve *b*), and 10^{21} cm^{-3} (curve *c*), respectively. The dashed line is the result of our previous analysis (Ref. 3) of the electron-transmission experiments in solid Xe films at 45 K. The energy of the bottom of the conduction band is chosen as the zero energy.

be made here regarding our estimated concentration of defects (2—3 %) which may seem somewhat high for rare-gas samples. As mentioned in Ref. 9, under the experimental film growth conditions of Ref. 2 (45 K and 10^{-10} Torr), high vacancy concentrations are expected to be formed. Our 2—3 % concentration of defects should likely reflect the presence of these vacancies in the studied films. However, such a value might also be somewhat overestimated since we ignored in the calculations the scatterings due to impurities, grain boundaries, and other kinds of structural imperfections which can also be present in the experimental films. It is clear that any contribution from these scattering mechanisms would decrease our estimated concentration of defects, which should in turn be regarded as an upper limit value.

The conclusions of this work are as follows: (i) the main mechanisms responsible for the scattering of incident electrons in thin solid Xe films used in electron-transmission experiments are due to acoustical phonons and to neutral point defects, (ii) the oscillating behavior of the electron MFP as a function of energy is entirely determined by the changes in the electron effective mass with energy, and (iii) low-energy electron-transmission experiments in the elastic scattering region offer a valuable tool for getting information about the variation of the electron effective mass with energy in solids.

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*Also at Centre de Recherche en Physique du Solide, Département de Physique, Faculté des Sciences, Université de Sherbrooke, Sherbrooke, Québec, Canada J1K 2R1.

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