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HOLE-PHONON SCATTERING AND THERMAL CONDUCTIVITY OF *p*-TYPE InSb FROM 2 TO 100 K

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Abstract

The hole-phonon interaction contributing to the thermal conductivity of three *p*-type samples of InSb is analyzed between temperatures of 2 and 100 K. In addition to the phonon scattering by bound and free holes, other phonon scattering such as boundary, point defect and phonons are considered. Both relaxation rates for $q \leq 2k_F$ and for $q > 2k_F$ are used for free hole-phonon scattering. The role of screening due to plasma on hole-phonon scattering is also included. The Callaway model for thermal conductivity is utilized from which an excellent fit to the experimental data is obtained over the whole temperature range.

Keywords: hole-phonon scattering, *p*-type InSb, thermal conductivity

Introduction

Indium antimonide is a III–V compound semiconductor with the zincblende structure and is a member of the InX family of compounds where *X* may be N, P, As or Sb. The temperature dependence of the thermal conductivity of *p*-type InSb has been extensively investigated by several workers [1–5]. Previously Challis *et al*. [1] gave a qualitative discussion based on electron–phonon scattering in *p*-type InSb. They indicated that such scattering occurs at heavily doping concentrations. The reduction in the thermal conductivity of doped semiconductors at low temperatures is attributed to the scattering of phonons by holes (electrons) [6–11]. The free hole (electron)-phonon scattering relaxation rate was given by Ziman [12] and modified by Kosarev [3], who took into account the effect of the electric field due to ionized atoms. That means that phonons with wave vector exceeding $2k_F$ can also contribute to the hole-phonon scattering. In their attempt to explain the temperature dependence of the thermal conductivity of highly doped *p*-type InSb at helium temperatures, Crosby and Grenier [2] included the effect of screening due to the hole system acting as a plasma. Singh [11] tried to explain the phonon conductivity of highly doped HgTe by considering the effect of the plasma screening and also the electric field due to ionized atoms. Singh and Verma [13] and Singh [14] also found that this mechanism is quite successful in explaining the phonon conductivity of highly doped *p*-type GaAs and InSb and

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n-type Ge and Si respectively. It is noted that the impurity states in semiconductors can be classified into low, intermediate and high concentrations respectively. For low concentrations, the holes are bound to impurity states or in nonmetallic state and at high concentrations they are free or in metallic state, and for the samples with intermediate concentration both the free and bound holes are found [15].

In the present paper, for scattering of phonons by bound holes the theory of Suzuki and Mikoshiba [7] seems to be valid for this case. The scattering of phonons by free holes has been treated by using a modified Ziman model by Crosby and Grenier [2] and Kosarev [3]. Thus the hole-phonon scattering relaxation rate is taken as a sum of the relaxation rate due to the scattering of phonons by free and bound holes. Based on Mikoshiba [15] 'inhomogeneity model' the number of holes in the metallic and nonmetallic region can be calculated for each sample. Following the above relaxation rates, the purpose of this paper is to calculate the thermal conductivity of doped *p*-type InSb in the temperature range from 2 to 100 K and with impurity concentrations from $5.3\cdot10^{15}$ to $6\cdot10^{18}$ atoms per cm^3. We have mentioned other scattering processes earlier such as boundary, point defect and phonon-phonon scattering. The relaxation rates of these scattering processes are used in the Callaway's expression of thermal conductivity. To analyze the influence of screening on hole-phonon scattering, we have computed the thermal conductivity with and without the effect of screening. A brief discussion is presented on the phonon scattering frequencies due to the four principal scattering mechanisms.

Theory

Expression for hole-phonon scattering

In heavily doped *p*-type semiconductors, the impurity level lies within the valance band, so holes are considered to be free. According to Ziman [12] who used the effective mass approximation, the relaxation rate for the scattering of phonons by free holes (electrons) can be expressed as

$$\tau_{\text{fh}}^{-1}=axTF(x) \quad \text{for } q\leq 2k_{\text{F}} \tag{1}$$

$$\tau_{\text{fh}}^{-1}=0 \quad \text{for } q>2k_{\text{F}} \tag{2}$$

where

$$a=\frac{C^2(m^*)^2K_{\text{B}}\eta^2}{4\pi\hbar^4\rho v},\quad k_{\text{F}}=(3\pi^2N_{\text{m}})^{1/3},\quad F(x)=\frac{1}{x}\ln\frac{\exp\left(\frac{x}{2}\right)+\exp(P)}{\exp\left(-\frac{x}{2}\right)+\exp(P)},$$

$$P=-\frac{T}{16T_{\text{s}}}\left[\left(\frac{\theta^*}{T}\right)^2-x^2\right],\quad \theta^*=\frac{2k_{\text{F}}\hbar v}{K_{\text{B}}},\quad T_{\text{s}}=\frac{0.5mv^2}{K_{\text{B}}},\quad x=\frac{\hbar\omega}{K_{\text{B}}T},\quad \eta=\vec{q}\vec{e}$$

C is the dilatation deformation potential, m^* is the effective hole mass, v is the phonon velocity, ρ is the mass density, $\bar{e}$ is the polarization vector, $\bar{q}$ is the phonon wave vector, k_F is the radius of the hole Fermi surface, θ^* is called the effective Debye temperature and N_m is the number of free holes.

Kosarev [3] pointed out that when the influence of the electric field of the ionized impurity in which the hole-phonon scattering takes place is included, the limitation $q \leq 2k_F$ can be lifted. Therefore, phonons with wave vector $q > 2k_F$ can also interact with holes, and the scattering relaxation rate of such mechanism is written as

$$\tau_{fh}^{-1} = \frac{59\pi C^2 \eta^2 (m^*)^2 N_m \hbar^2}{R_B^3 \rho x^5 T^5 K_B^5}, \quad \text{for } q > 2k_F \tag{3}$$

where $R_B = (\hbar^2 \varepsilon)/(m^* e^2)$ is the effective Bohr radius, e is the electronic charge and ε is the dielectric constant.

It is expected that under qualitative consideration, the linear term $\tau_{fh}^{-1} = axt$ at low temperatures overestimates the scattering of the low q-phonon. When the phonon wave length is approximately equal or greater than the carrier mean free path, a decrease in the strength of the scattering should take place. A decrease in the phonon–electron scattering is also expected at low frequency phonons due to the behaviour of the electron system as a plasma. The screening function is given by Crosby and Grenier [2] to have the form

$$S(x) = \left[1 + 3\left(\frac{q_{TF}}{q}\right)^2\right]^2 \tag{4}$$

Here $q_{TF} = ((4\pi N_m e^2 m^*)/(\varepsilon \hbar^2 k_F^2))^{1/2}$ is the Thomas–Fermi wave vector. Hence the total effective free hole-phonon scattering relaxation rate reduces to

$$\tau_{fh}^{-1} = \frac{\tau_{fh}^{-1}(q \leq 2k_F)}{N(x)} + \frac{\tau_{fh}^{-1}(q > 2k_F)}{S(x)} \tag{5}$$

Following the work of Suzuki and Mikoshiba [7], the relaxation rate for the scattering of phonons by bound holes can be given by

$$\tau_{bh}^{-1} = \frac{N_n \omega_q^2}{100\pi \rho^2 \hbar^2 v^2} \left(\frac{2}{3} D_{u'}^a\right)^4 f^2 \frac{\omega_q}{v} \left[\frac{1}{v_L^5} f^2\left(\frac{\omega_q}{v_L}\right) + \frac{3}{2}\frac{1}{v_T^5} f^2\left(\frac{\omega_q}{v_T}\right)\right] W_t \tag{6}$$

where

$$\begin{aligned} W_1 &= 24 + 48D^2 + 8D^4, \\ W_2 &= 16 + 37D^2 + 7D^4, \\ W_3 &= 20 + 35D^2 + 5D^4, \end{aligned} \tag{7}$$

$$D=\frac{D_{u}^{a}}{D_{u'}^{a}} \quad \text{and} \quad f(q)=\left(1+\frac{1}{4}R_{B}^{2}q^{2}\right)^{-2}$$

In these expressions N_n is the number of bound holes, v_L and v_T are the velocities for longitudinal and transverse phonons respectively, D_u^a and $D_{u'}^a$ are referred to the shear deformation potential. Thus the total hole-phonon scattering relaxation rate becomes

$$\tau_{hp}^{-1}=\tau_{fh}^{-1}+\tau_{bh}^{-1} \tag{8}$$

Inhomogeneity model have previously been presented by Mikoshiba [15], who gave a phenomenological treatment from which the impurity states in semiconductors can be classified into three cases: low, intermediate and high concentrations. He tried to explain the properties of the intermediate concentration by supposing the impurity states as spatial mixtures of metallic and non-metallic regions. In the frame of this model, the number of impurities in the metallic (N_m) and nonmetallic state (N_n) can be expressed as

$$N_{m}=N\left[1-\exp\left(-\frac{4\pi}{3}Nr^{3}\right)\right] \tag{9}$$

$$N_{n}=N\exp\left(-\frac{4\pi}{3}Nr^{3}\right) \tag{10}$$

where N represents the number of the present impurities and $r=(144/\pi^2)^{1/3}R_B$.

Expression for the thermal conductivity

The thermal conductivity, according to Callaway [16], can be expressed as

$$K=\frac{K_{B}}{2\pi^{2}v}\left(\frac{K_{B}T}{\hbar}\right)^{3}\int_{0}^{\theta_{D}/T}\tau_{c}x^{4}e^{x}(e^{x}-1)^{-2}\mathrm{d}x+\Delta K \tag{11}$$

Here θ_D is the Debye temperature and v, the average velocity obtained from the longitudinal and transverse phonon velocities, is given by

$$\frac{1}{v}=\frac{1}{3}\left(\frac{1}{v_{L}}+\frac{2}{v_{T}}\right) \tag{12}$$

In above equation, τ_c^{-1} is the combined scattering relaxation rate is given by

$$\tau_{c}^{-1}=\tau_{B}^{-1}+\tau_{pt}^{-1}+\tau_{3ph}^{-1}+\tau_{hp}^{-1} \tag{13}$$

where τ_B^{-1}, τ_{pt}^{-1} and τ_{3ph}^{-1} are the relaxation rates due to the scattering of phonons by boundary, point defects and phonons, respectively.

The boundary scattering relaxation rate, which is based upon the work of Casimir [17], is taken to be $\tau_B^{-1}=v/(1.12F\sqrt{s})$. Where s is the cross-section area of the sample and F is related to the fraction of the phonons which are diffusely scattered at the boundary. According to Ziman *et al*. [18], F measures the effect of finite sample length.

For Raleigh scattering by point defects, the expression for the relaxation rate used is [19]

$$\tau_{pt}^{-1}=A\omega^4 \tag{14}$$

τ_{3ph}^{-1} is the three phonon scattering relaxation rate and is given by [16]

$$\tau_{3ph}^{-1}=B\omega^2T^3 \tag{15}$$

where A and B are the scattering strength of the respective scattering processes. They are treated as adjustable parameters, which can be evaluated from the best fit between the theoretical and experimental values of thermal conductivity. τ_{hp}^{-1} is the relaxation rate for hole-phonon scattering given in Eqs (1)–(8).

ΔK is the correction term due to the three phonon normal processes. The author [20, 21] found that the contribution of the correction term is usually small enough in comparison with the total thermal conductivity and can be ignored.

Results and discussion

The values of the various parameters used in the analysis of thermal conductivity between 2 and 100 K with concentration range $5.3\cdot10^{15}$–$6.0\cdot10^{18}$ cm^{-3} are listed in Tables 1 and 2. Using Eqs (9) and (10), the concentration of acceptor holes in the metallic (free) and nonmetallic (bound) region are cited in Table 3. The theoretical curves of $K(T)$ of p-type InSb are shown in Figs 1–3 together with the experimental data given by Kosarev *et al*. [4]. The theoretical curves have been calculated with the help of the numerical analysis of Eq. (11). The variation of screening function ($S(x)$) with the dimensionless variable x is classified in Fig. 4. The variation of the scattering relaxation rates with the dimensionless variable x is plotted in Figs 5–7 at T=2 K for different carrier concentrations to show the domination of one over other scattering relaxation rates. The values of F, A, B, C, D_u^a and $D_{u'}^a$ are treated as adjustable parameters obtained for the best fit to the experiment.

For the boundary scattering relaxation rate, the correction factor F is related to the fraction f of phonons which are diffusely scattered at the boundaries according to $F=(2–f)/f$. For completely diffused scattering F=1 is taken and larger than unity if part of the phonons are specularly reflected. In the present investigation, the values of F for different samples lie between 1.0 and 1.84. These values are fairly acceptable.

In the hole-phonon scattering relaxation rate, η=1 is considered because the longitudinal phonons are the main scatterers of phonons [24], which is in accordance with the prediction of other workers [11, 24–27]. For samples 9 and 8b, the values of the effective Debye temperatures θ^* and Thomas–Fermi wave vector q_{TF} are determined from the measured carrier densities, while for sample 7b were treated as adjustable parameters to fit the experiment. Crosby and Grenier [2] for p-InSb and

Singh [11] for *p*-HgTe have treated them as adjustable parameters. The values of q_{TF} obtained by curve fitting are much smaller than those calculated from the carrier density.

Table 1 Physical parameters used in the calculation

Parameter	Value	Reference
ρ/g cm^{-3}	5.775	[22]
v/cm s^{-1}	$2.375 \cdot 10^{5}$	
v_L/cm s^{-1}	$3.8 \cdot 10^{5}$	[3]
v_T/cm s^{-1}	$2.0 \cdot 10^{5}$	[3]
θ_D/K	172.5	[23]
m^*	0.4	[22]
R_B/A	23.8	
ε	18	[22]
η	1	

Table 2 Values of the parameters obtained by adjustment for the best fit between the experiment and theory. The numbers in parentheses are calculated from the impurity concentration

	Sample 9	Sample 8b	Sample 7b	
S/mm^2	2.76×2.95	1.13×1.34	1.23×1.39	
F	1.84	1.0	1.1	
C/eV	11.87	11.87	11.87	
A/s^3	$7.0 \cdot 10^{-44}$	$3.5 \cdot 10^{-44}$	$3.2 \cdot 10^{-44}$	
B/s K^{-3}	$1.1 \cdot 10^{-22}$	$1.5 \cdot 10^{-22}$	$1.0 \cdot 10^{-22}$	
D_u^a/eV	0.3	0.7	0.7	
$D_{u'}^a$/eV	0.4	1.0	1.0	
q_{TF}/cm^{-1}	$(3.17 \cdot 10^{6})$	$(1.95 \cdot 10^{6})$	$(3.97 \cdot 10^{5})$	$8.4 \cdot 10^{4}$
θ^*/K	(20.35)	(7.69)	(0.32)	1.5
$2k_F$/cm^{-1}	$(1.12 \cdot 10^{7})$	$(4.24 \cdot 10^{6})$	$(1.922 \cdot 10^{5})$	$8.26 \cdot 10^{5}$

Table 3 Concentrations of free and bound holes

	N/cm^{-3}	N_m/cm^{-3}	N_n/cm^{-3}
Sample 9	$6.0 \cdot 10^{18}$	$5.957 \cdot 10^{18}$	$4.3 \cdot 10^{16}$
Sample 8b	$7.2 \cdot 10^{17}$	$3.23 \cdot 10^{17}$	$3.97 \cdot 10^{17}$
Sample 7b	$5.3 \cdot 10^{15}$	$3.0 \cdot 10^{13}$	$5.27 \cdot 10^{15}$

Applying the screening effect, the value of the dilatation deformation potential C seems to be independent of the impurity concentration, while the shear deformation potential is found to be of varying value. It should also be noted that Singh [11] applied the same value for C for both samples of p-HgTe, while Crosby and Grenier [2] found a very slight dependency of the deformation potential on the impurity concentration of p-InSb. The obtained values of the deformation potential are within the range expected [28, 29].

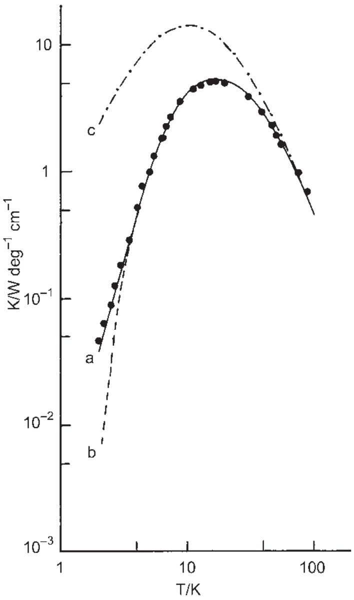

Fig. 1 Plot of thermal conductivity *vs*. temperatures for p-type InSb sample 9, solid line: calculated; circles: experimental values

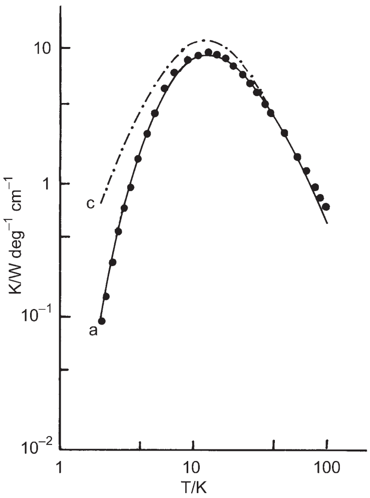

Fig. 2 Plot of thermal conductivity *vs*. temperatures for p-type InSb sample 8b, solid line: calculated; circles: experimental values

Figures 1–3 reveal an acceptable fit, as shown by the continuous lines (curve a) to the whole temperature range of the experimental curve. These figures indicate that the present model which considers that the holes exist in both bound and free states is quite successful in explaining the thermal conductivity of *p*-InSb. These figures also show the effect on the thermal conductivity arising from the absence of: (b) the screening effect ($S(x)$=1) and (c) the hole-phonon scattering $\tau_{hp}^{-1}=0$. One can see from curves (b) and Fig. 4 that the effect of screening due to plasma is more important at

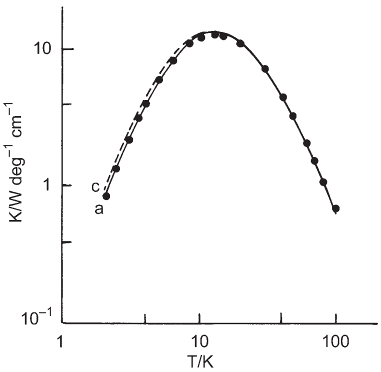

Fig. 3 Plot of thermal conductivity *vs*. temperatures for *p*-type InSb sample 7b, solid line: calculated; circles: experimental values

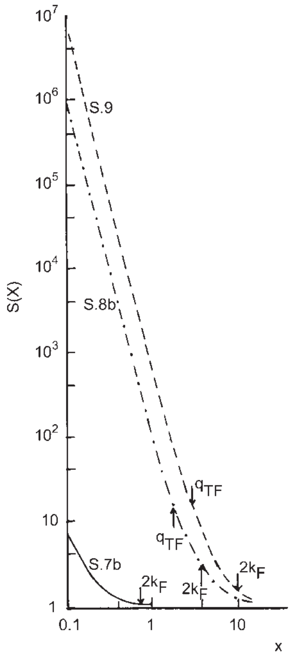

Fig. 4 The variation of the screening function $S(x)$ with the dimensionless parameter x

low temperatures (T<4 K) in the case of sample 9 and it is minor in case of samples 8b and 7b. In other words, the effect of screening is more important in the heavily doped sample (sample 9) when compared with lightly doped samples (samples 8b and 7b). At the same time, with the help of Fig. 4, it can also be confirmed that the screening effect decreases with increasing phonon frequency. Just below the value of Thomas–Fermi wave vector q_{TF}, it can be noted that the screening effect changes rapidly downward, while above this it shows a slow variation with the dimensionless variable x. Above $2k_F$, it becomes clear that the screening effect tends to unity ($S(x)=1$). As a result, it can be concluded that when the order of the phonon wave length equal or becomes larger than Thomas–Fermi wave length (i.e. $q \leq q_{TF}$) a sharp fall in the strength of the hole-phonon scattering should happen. Also one can conclude that the plasma screening becomes unimportant at $q>2k_F$. It should be mentioned that the Thomas–Fermi wave vector plays a remarkable role in reducing the amount of screening when it decreases. From the above analysis, it is expected that to reduce the effect of screening ($S(x)=1$) at $q>2k_F$, the restriction $2k_F>q_{TF}$ is required.

As it can be seen from curves (c), the hole-phonon interaction becomes effective at low temperatures, i.e. T<80 K in sample 9, T<40 K in sample 8b and T<10 K in sample 7b. It can also be seen that the hole-phonon interaction displays an increasing tendency as the impurity concentration increases.

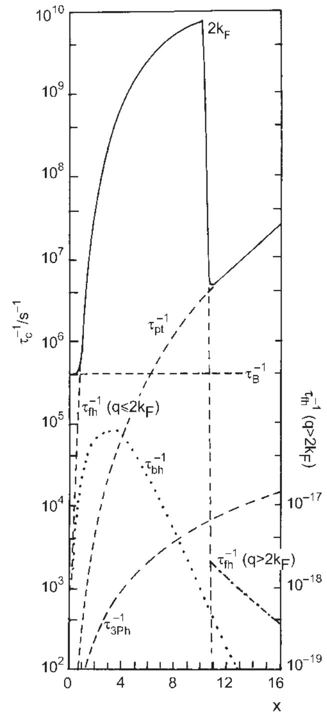

Fig. 5 Combined scattering relaxation rate as a function of dimensionless parameter x for p-type InSb sample 9 at 2 K

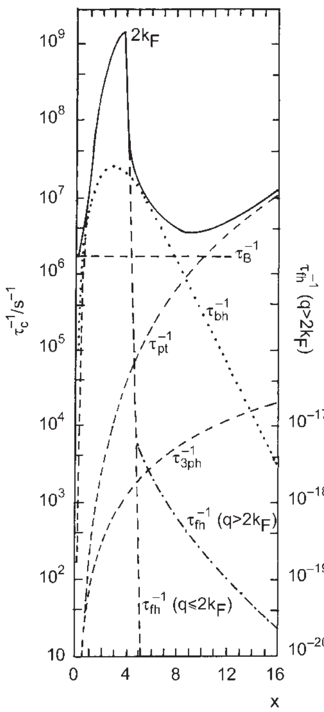

Fig. 6 Combined scattering relaxation rate as a function of dimensionless parameter x for p-type InSb sample 8b at 2 K

Figures 5–8 illustrate that for low value of x, the hole-phonon scattering dominates over other types of scattering. This reflects the effectiveness of the hole-phonon scattering at low temperatures. These figures show that when $q \leq q_{TF}$, the carrier scattering exhibits a very rapid fall. This is undoubtly attributed to the presence of the screening effect. They also demonstrate a very drastic cutoff of hole-phonon scattering at $2k_F$. We would like to comment on the variation of free hole-phonon scattering relaxation rate τ_{fh}^{-1} for $q>2k_F$. As far as we know, $R_B \propto (m^*)^{-1}$, where m^* is the hole mass, and from Eq. (3) $\tau_{fh}^{-1}(q>2k_F) \propto (m^*)^5$. Since the effective mass is small for p-type InSb, a decrease in τ_{fh}^{-1} (q>2k_F) is expected. It becomes ineffective, indicating that the thermal conductivity can be calculated by taking only Ziman scattering (τ_{fh}^{-1}(q>2k_F)) cited in Eq. (8). From Figs 5–8, it can be easily seen that at low frequency, the bound hole-phonon scattering decreases to ω_q^2 with decreasing frequency, and for all the three samples reaches its maximum value at $\omega \approx 7.85 \cdot 10^{11}$ s^{-1}. For large values of x (i.e. x>11), τ_{pt}^{-1} dominates over other scattering relaxation rates, but for such values of x, the integral stated in Eq. (11) has a very low value due to the factor $x^4e^x(e^x-1)^{-2}$ (Fig. 8).

To summarize, in the present theoretical work the variation of the thermal conductivity of p-type InSb with temperatures between 2 and 100 K has been investigated by a completely different approach. This approach, instead of considering the acceptor holes to be free in the valance band for all concentrations of impurities, it assumes the acceptor holes exist in both free and bound states. For bound holes the relaxation rate for hole-phonon scattering given by Suzuki and Mikoshiba [7] is used, while scattering of phonons by free holes is treated using the Ziman model as modified by Crosby and Grenier [2] and Kosarev [3].

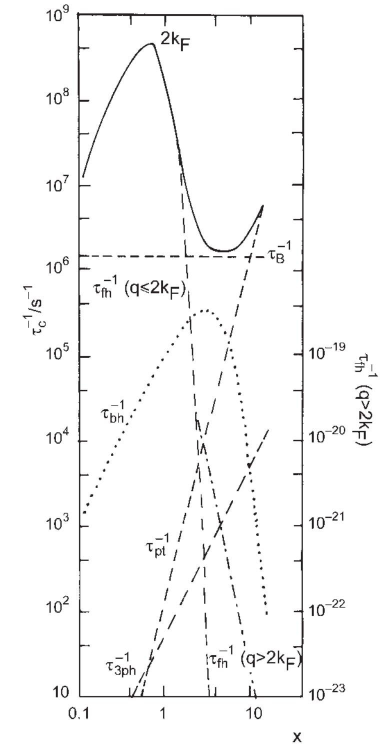

Fig. 7 Combined scattering relaxation rate as a function of dimensionless parameter x for p-type InSb sample 7b at 2 K

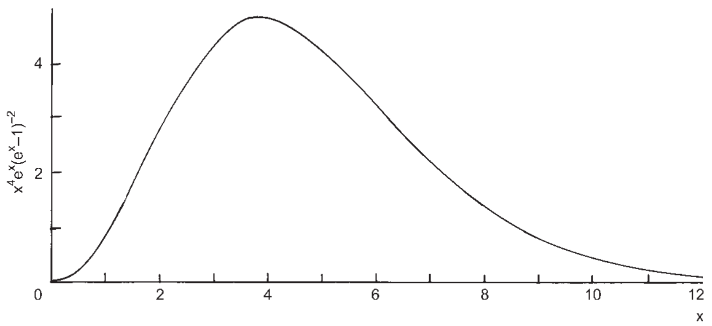

Fig. 8 The variation of the factor $x^4e^x(e^x–1)^{-2}$ with the dimensionless parameter x

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