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The Effect of the Three Phonon Scattering on the Phonon Drag Thermoelectric Power of As and Sb-Doped Ge

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ABSTRACT. The effect of the three phonon scattering on the phonon drag thermoelectric power of As and Sb doped Ge has been studied in the temperature range 2-20K.

At very low temperatures, it is found that the effect of the Umklapp processes are very small and can be ignored while the Normal processes are in a good agreement with the calculated values up to 10K. Above 10K both kinds of scatterings should be included in the calculations.

The study has shown that the most important scattering mechanisms in such samples are the electron-phonon and the point-defects scatterings.

The phonon-phonon scattering is playing an important role in energy transfer of semiconductors. Due to the complex structure of the Brillouin zone and the strong temperature dependence of the phonon distribution function, the relaxation rate (τ_{3ph}^{-1}) has a complicated expression.

It is well known (Klemens 1965, Callaway 1959, Gaur and Sand Verma 1967, Guthrie 1960), that the phonon-phonon scattering processes can be divided into two groups: normal processes (N-processes) in which momentum is conserved and umklapp processes (U-processes) in which momentum is not conserved. It should be noted that the four phonon processes have been ignored in this study because they are important at high temperature only (Dubey 1980).

In spite of the fact that the three phonon scattering processes dominate over the other processes at high temperatures, these processes are not small at low temperatures.

Several workers have proposed different expressions for τ_{3ph}^{-1}, and different for transvers and longitudinal phonons. To discuss the dependence of τ_{3ph}^{-1} on the temperature T and the phonon frequency ω, Callaway (1959), used ω for the transvers phonons and ω^2 for longitudinal phonons respectively. Herring (Bearman 1976) used the expression τ_{3ph}^{-1} ωT^4 for N-processes which takes place by the transvers phonons and τ_{3ph}^{-1} $\omega^2 T^3$ for the longitudinal phonon. Klemens (1958) calculated the three phonon scattering relaxation rate for the U-processes as τ_{3phU}^{-1} $g(\omega)f(T)\exp(-\theta/\alpha T)$ where $g(\omega)$ is the phonon frequency function, α is a constant and θ is the Debey temperature.

Table 1 contains these scattering relaxation rates together with the other scattering relaxation rates used in the present study. The undefined terms will be explained later.

At very low temperatures, it is well established that the Callaway expression for the scattering relaxation rate for the N-processes τ_{3phN}^{-1}, and the Klemens expression for the U-processes τ_{3phU}^{-1} are in a good agreement with the experimental data. These scattering relaxation rates have been used to study the effect of τ_{3ph}^{-1} on the phonon drag thermoelectric power (PDTEP) of As and Sb doped Ge in the temperature range 2-20K.

Scattering Relaxation Rates and the PDTEP Integral

Recently, Saif and Dubey (1990) studied the PDTEP of six samples of As and Sb doped Ge in the temperature range 2-20K. These samples were selected from the earlier report of Goff and Pearlman (1965). The three phonon scatterings have not been included because of the difficulties in the calculations.

The calculated thermoelectric power of the doped semiconductors can be considered as the sum of two contributions, the first which is due to electrons and called the electronic thermoelectric power (ETEP) and the other, which is due to the phonon drag and called the phonon drag thermoelectric power (PDTEP). It is well known, (Goff and Pearlman 1965), that the latter is most important, at low temperatures, than the other.

According to Klemens (1969) and Sondheimer (1956), the PDTEP can be expressed as:

$$Q_{PH} = \frac{3k}{e}\left(\frac{T}{\theta}\right)^3 \int_0^{\theta/T} \frac{f(\tau)\, x^4 \exp(x)}{(\exp(x)-1)^2}\, dx \qquad (1)$$

where k is the Boltzman constant, e is the electronic charge, θ is the characteristic temperature (which differentiates non-peripheral phonons from peripheral

phonon, see (Dubey 1980)) $\hbar$ is the Planks constant divided by two π, $x = \hbar\omega/kT$, T is the absolute temperature, ω is the phonon frequency, $f(\tau)$ is the scattering function with depends on the scattering relaxation rates.

In dopped semiconductors, the phonon scatters are the electrons, crystal boundaries, point-defects and other phonons. The scattering function $f(\tau)$ can be expressed as the sum of the scattering relaxation rates due to the different scattering mechanisms (Goff and Pearlman 1965), hence

$$f(\tau) = \tau_{ep}^{-1} (\tau_{ep}^{-1} + \tau_B^{-1} + \tau_{pt}^{-1} + \tau_{3ph}^{-1})^{-1} \quad (2)$$

where τ_{ep}^{-1}, τ_B^{-1} and τ_{pt}^{-1} are the scattering relaxation rates due to the scattering of phonons by electrons, crystal boundaries and point-defects respectively. These scattering relaxation rates have been calculated by using expression introduced by Ziman (1960), Casimir (1938) and Klemens and Ecsedy (1976) respectively. These scattering relaxation rates are.

$$\tau_{ep}^{-1} = DT \ln[(1+\exp(R+x/2))/(1+\exp(R-x/2))] \quad (3)$$

$$\tau_B^{-1} = \upsilon/L \quad (4)$$

$$\tau_{pt}^{-1} = A\omega^4 \quad (5)$$

where $D = E_e^2 m^{*2} k/4\pi\hbar^4 \rho\upsilon_l$

$$R = \eta^* - N/T - PTx^2$$

$$N = \tfrac{1}{2}m^* \upsilon_l^2/k$$

$$\eta^* = \varepsilon_f/kT$$

$$P = k/8m^*\upsilon_l^2$$

$$A = 3c_p a^3/\pi \upsilon^3$$

all the terms have there meaning as in the stated references.

Effect of τ_{3ph}^{-1} on the PDTEP of As and Sb Doped Ge

Two samples of Ge doped by As and Sb (As 226 and Sb 30 of Goff and Pearlman 1965), have been used to calculate the effect of τ_{3ph}^{-1} on the PDTEP. The electronic concentration of the samples used are $8.8. \times 10^{23}$ m^{-3} and 2.5×10^{24} m^{-3} respectively. Table 2 contains the constants that have been used to calculate the PDTEP in the temperature range 2–20K. Using these constants and numerical integration of equation (1), the variation of the PDTEP with the temperature for As-Ge and Sb-Ge are shown in Fig. 1 and Fig. 2 respectively. One

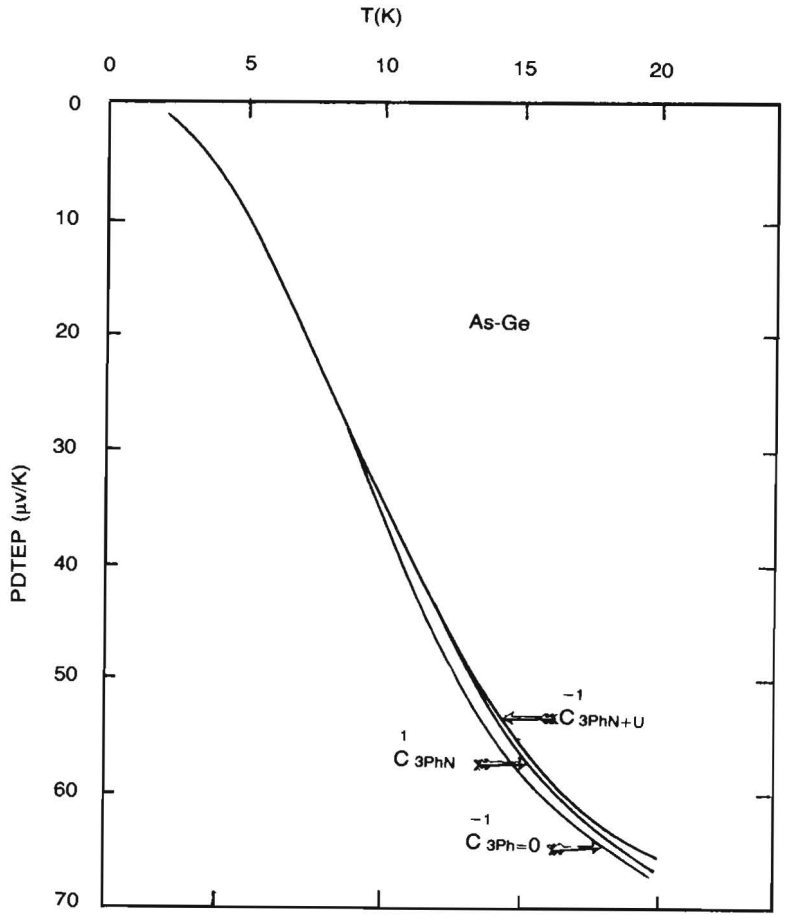

Fig. 1. The phonon drag thermoelectric power of As doped Ge in the temperature range 2-20K for the case of using.

can see from these figures that the effect of the normal and umklapp processes, in both samples, is very small in the temperature range 2−8K. One can attribute this behaviour to the dominating nature of τ_B^{-1} and τ_{ep}^{-1} where most of the phonons undergo scattering by the crystal boundaries and the electrons of the sample which are of high concentration (more than 10^{23} m^{-3}).

At temperature above 8K, the curve for the τ_{3phN}^{-1} and τ_{3phN+U}^{-1} shows deviation from the curve for the $\tau_{3ph=0}^{-1}$ which is considered as our reference as shown in figures 1 and 2. At temperature above 15K, the difference in the value

from the reference curve for the τ_{3phN}^{-1} and τ_{3phN+U}^{-1} become noticeable.

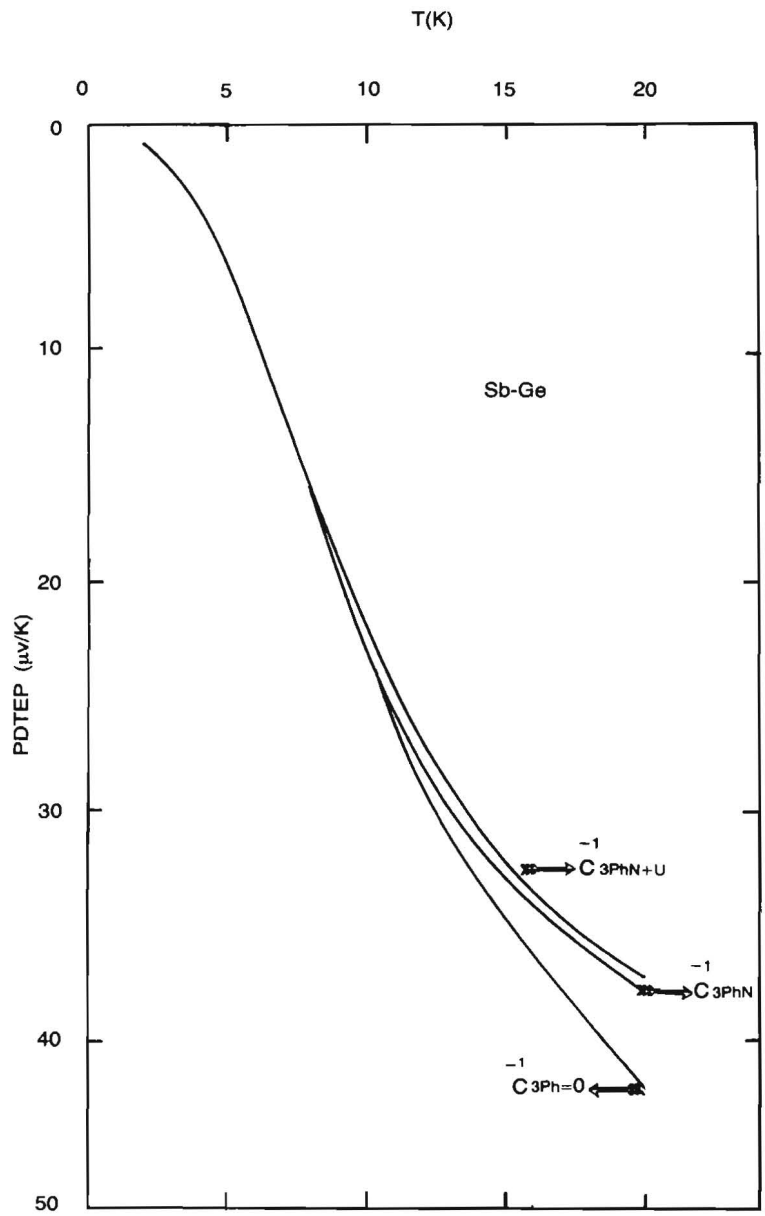

Fig. 2. The phonon drag thermoelectric power of Sb doped Ge in the temperature range 2-20K for the case of using.

One can attribute the deviation from the reference curve at the temperature range 8–15K to the low momentum scattered phonons, where most of the scattering processes are N-processes. While at higher temperatures, the reason for the deviation from the reference curve is attributed to the scattering mechanisms of the both kinds (N and U-processes).

Table 1. Relaxation rates at low temperatures (for the meaning of the terms see references)

Scattering process	**Relaxation rate**
three-phonon	
Normal process Bearman (1976) τ_{3phN}^{-1}:	
longitudinal	$B_L\omega^2T^3$
transverse	$B_T\omega T^4$
Umklapp process τ_{3phU}^{-1}	
Klemens (1958)	$B_U\omega^2T^3e^{-\theta/\alpha T}$
Klemens (1976)	$B_U\omega T^3e^{-\theta/\alpha T}$
Callaway (1959)	$B_U\omega^2T^3$
Electron-phonon (Ziman (1960) τ_{ep}^{-1}	$(E^2m^{*2}kT/4\pi h\rho v_l)$ ln $(1+\exp(R+x/2)/(R(x/2))$
Point-defects Klemens (1976) τ_{pt}^{-1}	$A\omega^4$
Crystal boundary Casimir (1938) τ_B^{-1}	v/l

Table 2. The constants used in the study of the PDTEP of As, Sb doped Ge in the temperature range 2-20K

	Sb 30	**As 226**
n (m^{-3})	2.5×10^{24}	8.8×10^{23}
θ^* (K)	46	40
τ_B^{-1} (10^5 Sec^{-1})	15.80	8.81

θ = 376 K
v = 3.9×10^3 $m.S^{-1}$
v_1 = 4.92×10^3 $m.S^{-1}$
B_N = 5.0×10^{-23} $Sec.deg^{-3}$

The percentage correction, that should be made to the value of the PDTEP in the case of neglecting τ_{3phU}^{-1} and τ_{3phN}^{-1} has been calculated and is reported in Table 3.

Table 3. The percentage correction of the PDTEP of As and Sb doped Ge in the temperature range 2-20K

T(K)	As 226		Sb 30	
	$\%Q(\tau_{3phN}^{-1})$	$\%Q(\tau_{3phU}^{-1})$	$\%Q(\tau_{3phN}^{-1})$	$\%Q(\tau_{3phU}^{-1})$
2	0.00	0.00	0.00	0.00
4	0.00	0.40	0.00	0.35
6	0.00	1.20	0.00	1.90
8	0.00	2.20	0.00	2.00
10	0.00	2.40	0.00	3.30
15	0.01	2.50	0.02	7.50
20	0.54	2.60	1.50	14.10

The values of the corrections shown in this table are very small below 10K. The correction is zero for the first case, so one can calculate the PDTEP by using rate τ_{3phN}^{-1} only. Above 10K, a correction should be made (especially for the second case $\tau_{3ph=0}^{-1}$) to obtain an agreement between the calculated and the experimental values of the PDTEP.

The scattering relaxation rates

Finally, we should discuss the scattering relaxation rates used in the present study. The variation of these scattering relaxation rates with the dimensionless variable $x = \hbar\omega/kT$ is shown in Fig. 3 for Sb 30 as an example. This figure shows that at values of $x<6$ the dominant scattering rates is τ_{ep}^{-1} because of the high concentration of electrons. While at the values of $x>6$ the dominate scattering relaxation rate is τ_{pt}^{-1} due to the factor $\times^4 e^{\times}(e^{\times}-1)^{-2}$. For a certain temperature, there is a value of $\times$ at which τ_{ep}^{-1} is zero, this value corresponds to the cut off phonon frequency of the peripheral phonons Saif and Dubey (1990). At all temperatures, τ_B^{-1} is a constant because it does not depends on $\times$, but it dominates at very low temperatures rather than the τ_{ph}^{-1} and τ_{pt}^{-1}.

Figure 3 also shows that τ_{3ph}^{-1} increases as $\times$ increases but still its value is less than the value of τ_{ep}^{-1} and τ_{pt}^{-1}.

Clearly, one notices that τ_{3phU}^{-1} has a small effect on the PDTEP than τ_{3phN}^{-1} due to the exponential factor $\exp(-\theta/\alpha T)$.

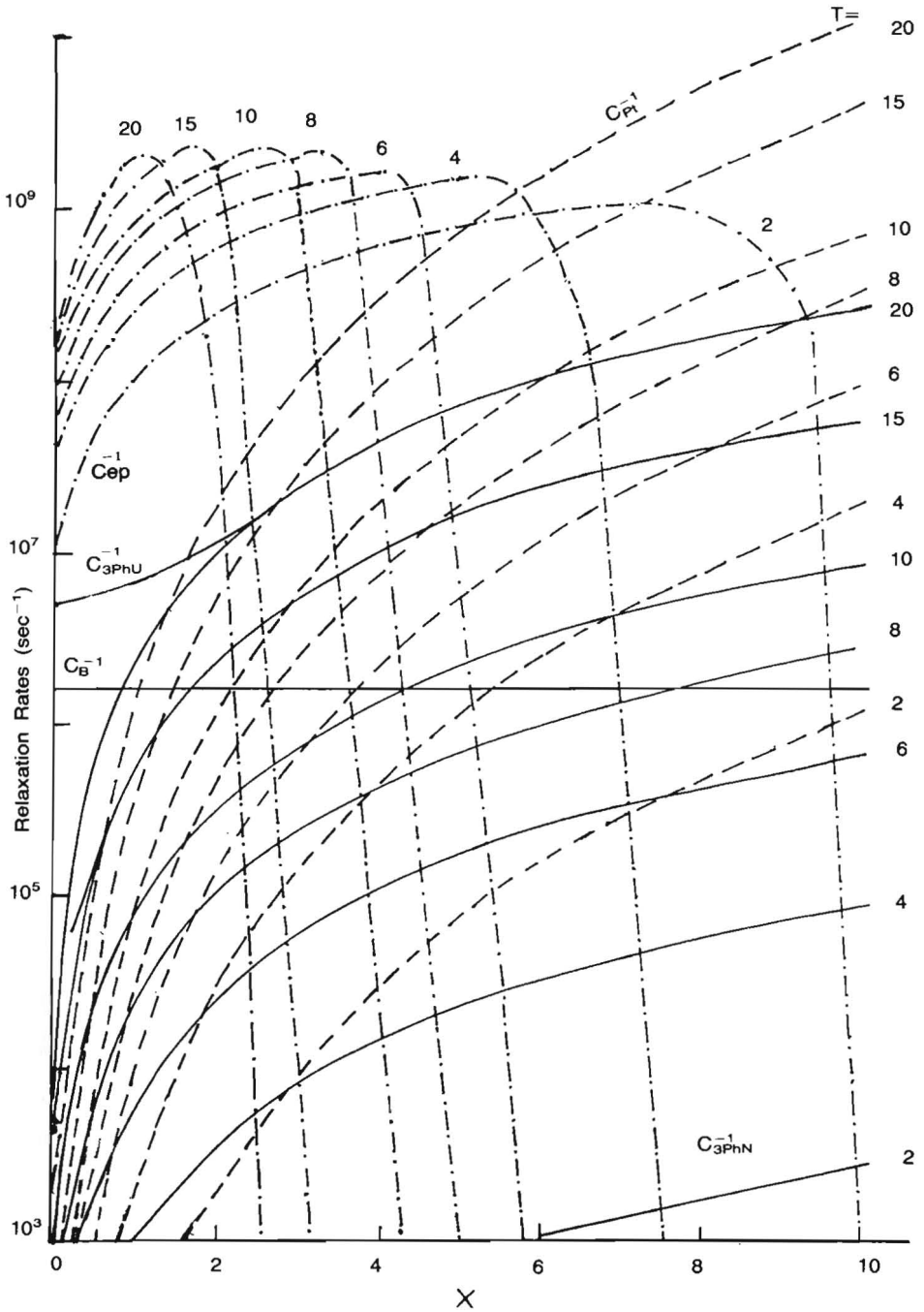

Fig. 3. The variation of scattering relaxation rates τ_{ep}^{-1}, τ_B^{-1}, τ_{pt}^{-1} and τ_{3ph}^{-1} with the dimensionless parameter $\times$ at a constant temperatures. Values stated near the curve represent temperatures.

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تأثير استطارة الفونون الثلاثية على الطاقة الحرارية ـ الكهربائية للفونون المقاوم للزرنيخ As والأنتيمون Sb المعالج بالجرمانيوم Ge

جلال صدام سيف و أ. هـ عوّاد

قسم الفيزياء ـ كلية التربية ـ جامعة البصرة ـ البصرة ـ العراق

لقد تم في هذا البحث دراسة تأثير استطارة الفونون الثلاثية على الطاقة الحرارية ـ الكهربائية للفونون المقاوم للزرنيخ والأنتيمون المعالج بالجرمانيوم وذلك ضمن المجال الحراري (٢ ـ ٢٠°) درجة مئوية.

من المعلوم أنه يوجد أسلوبين لاستطارة الفونون: الأول هو الأسلوب «N» وفيه تبقى كمية الحرارة مصونة، والثاني هو الأسلوب «U» وفيه لا تبقى كمية الحرارة مصونة. هذا ويمكن إعتبار الطاقة الحرارية ـ الكهربائية لأنصاف النواقل المعالجة بأنها حاصل جمع طاقتين.

الأولى: تعزى للإلكترونات، وتسمى الطاقة الحرارية ـ الكهربائية الإلكترونية ورمزها (ETEP).

الثانية: تعزى للفونون المقاوم وتسمى الطاقة الحرارية ـ الكهربائية للفونون المقاوم ورمزها (PDTEP).

لقد أخذت عينتان من As 226 و Sb 30 المعالجان بـ Ge لحساب تأثير معدَّل التراخي τ_{3ph}^{-1} على (PDTEP) ضمن شروط معينة.

ففي المجال الحراري (٢ ـ ١٠°) درجة، وُجد أن إستطارة الفونون بالأسلوب «U» صغيرة جداً ويمكن إهمالها، وأما استطارة الفونون بالأسلوب «N»

فهي متوافقة مع القيم المحسوبة (أنظر الشكلين ١ و ٢).

أمَّا من أجل المجال الحراري (١٠ ـ ٢٠°) درجة فقد وجد أنَّ كِلا أسلوبي استطارة الفونون ـ الأسلوب «U» والأسلوب «N» ـ يجب أن يدخلا في الحسابات.

هذا وتخلص الدراسة لإستنتاج أن القسم الأعظم من ميكانيكية الإستطارة في العينتين المذكورتين ناجمة عن إستطارة فونون ـ الكترون وإستطارة شوائب ـ نقطية.