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Magnetic field dependence of the "chemical shift" and the donor-electron radius in the lightly doped n-type Ge

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The present analysis of the resonance scattering of phonons by bound donors in As- and Sb-doped Ge in magnetic fields up to 78 kG applied along the [100] direction indicates that the "chemical shift" 4Δ increases with the magnetic field increase in the temperature range 1.3–4.4°K. At a field of 78 kG, the change is about 10%. The effective donor-electron radius also decreases by a factor of 15% for the same magnetic field. The above variations are in reasonable agreement with the calculations of Halbo for plots of $4\Delta/4\Delta_0$ and a/a_0 vs fields applied along the [100] direction, although in general the experimental shifts are lower than Halbo's theoretical values. The opposite effect of the increased magnetic field on the phonon conductivity is explained by the dominating role of 4Δ over a_0 causing an increase in the phonon conductivity of Ge(As) and a decrease in that of Ge(Sb). Universal curves for $4\Delta/4\Delta_0$ and a/a_0 vs H applied along the [100] direction have been obtained for the first time for Sb-, As-, and P-doped Ge.

I. INTRODUCTION

Recently we have investigated the role of compensating acceptor impurities[1] on the "chemical shift" 4Δ and the donor electron radius a_0 in n-type Ge. In this paper we propose to investigate the magnetic field dependence of the above two quantities. The basis of the present investigations are the expressions obtained by Suzuki and Mikoshiba[2] for the resonance scattering of phonons by bound donor electrons. The first successful theory for such a scattering was given by Griffin and Carruthers[3] and later on extended by Kwok,[4] who not only considered the elastic and inelastic scatterings but also phonon-assisted absorption processes. The donor-electron ground state is a singlet state and the next-higher-energy state is a triplet state, which is separated from the former by 4Δ, usually known as the chemical shift. The elastic and inelastic scatterings of phonons are considered both from the singlet as well as the triplet state.

For the present paper we have considered the magnetic field data of Sb- and As-doped Ge in the range 0–80 kG,[5] applied along a [100] direction. The temperature range in which the magnetic measurements have been carried out is from 1.3 to 4.4°K. The donor-electron concentration is 4.5×10^{16} cm^{-3} for As-doped Ge and 2.2×10^{16} cm^{-3} for Sb-doped Ge. However, the magnetic field causes opposite changes in the thermal conductivity of Sb- and As-doped Ge. In the former the conductivity decreases with the increase in the magnetic field whereas in the latter the conductivity increases with the increase in magnetic field. So far no quantitative explanation has been given for this effect.

An attempt has been made to explain the abovementioned anomalous results in the framework of Kwok's theory as extended by Suzuki and Mikoshiba. The calculations are based on the assumption that the magnetic field affects the donor-electron radius a_0 and the chemical shift 4Δ. The magnetic field shrinks the donor-electron wave function and hence the donor-electron radius, which represents the extent of the wave function, decreases. Since $\psi \propto a_0^{-3/2}$, the value of 4Δ increases with the decrease in the value of a_0. The present study of the resonant scattering of phonons in Sb- and As-doped Ge on the basis of the Suzuki and Mikoshiba (SM) expressions reveals that the effects of the magnetic field on a_0 and 4Δ are similar and approximately the same in both materials. The opposite effects of the magnetic field on the phonon conductivity are due to the dominating role of 4Δ causing an increase in the phonon conductivity of Ge(As) and a decrease in that of Ge(Sb) with the increase in magnetic field.

II. THEORY

The phonon conductivity K of the materials under consideration has been evaluated with the help of the following expression:

$$K(T)=\frac{k_B^4T^3}{6\pi^2\hbar^3}\sum_j\frac{1}{v_j}\int_0^\infty\frac{x^4e^x(e^x-1)^{-2}\,dx}{\tau^{-1}(q,j)}\ ,$$

where

$$\tau^{-1}(q,j)=\frac{v_j}{L}+A\left(\frac{k_B}{\hbar}\right)^4x^4T^4+(B_1+B_2)\left(\frac{k_B}{\hbar}\right)^2x^2T^5+\tau_{\mathrm{el}}^{-1}(q,j)+\tau_1^{-1}(q,j)+\tau_2^{-1}(q,j)\ ,$$

$$\tau_{\mathrm{el}}^{-1}(q,j)=B\omega^4(4\Delta)^2\{[(4\Delta)^2-\hbar^2\omega^2]^2+4\Gamma^2(4\Delta)^2\}^{-1}\ F(\omega)\{N_S(T)+N_T(T)[2+(4\Delta/\hbar\omega)^2]\}\ ,$$

$$\tau_1^{-1}(q,j)=\frac{B}{2}\,\omega\left[1-\exp\left(-\frac{\hbar\omega}{k_BT}\right)\right]\left(\frac{1}{\hbar\omega}-\frac{1}{4\Delta+\hbar\omega}\right)^2 N_T(T)\left(\frac{4\Delta}{\hbar}+\omega\right)^3 F\left(\frac{4\Delta}{\hbar}+\omega\right)\left[1-\exp\left(\frac{-4\Delta-\hbar\omega}{k_BT}\right)\right]^{-1},$$

$$\tau_2^{-1}(q,j)=\frac{B}{2}\,\omega\left[1-\exp\left(-\frac{\hbar\omega}{k_BT}\right)\right]\left(\frac{1}{\hbar\omega}+\frac{1}{4\Delta-\hbar\omega}\right)^2 N_S(T)\left|\frac{4\Delta}{\hbar}-\omega\right|^3 F\left(\frac{4\Delta}{\hbar}-\omega\right)\left[\exp\left(\frac{4\Delta-\hbar\omega}{k_BT}\right)-1\right]^{-1},$$

$$B=(\pi\rho^2\bar{v}_j^2)^{-1}(\tfrac{1}{3}\,\Xi_u)^4 f^2(\omega/\bar{v}_j)W_t\,,$$

$$F(x)\equiv\bar{v}_1^{-5}f^2(x/\bar{v}_1)+\tfrac{3}{2}\,\bar{v}_2^{-5}f^2(x/\bar{v}_2)\,,$$

$$W_1=\tfrac{48}{225}\,,\quad W_2=\tfrac{32}{225}\,,\quad W_3=\tfrac{40}{225}\,,$$

$$N_S(T)+3N_T(T)=1\,,\quad N_T(T)/N_S(T)=e^{-4\Delta/k_BT}\,,$$

$$\Gamma=\Gamma_S+\Gamma_T=\frac{1}{15\pi\rho}\left(\frac{\Xi_u}{3}\right)^2\left(\frac{4\Delta}{\hbar}\right)^3 F\left(\frac{4\Delta}{\hbar}\right)\left\{1+2\Big/\left[\exp\left(\frac{4\Delta}{k_BT}\right)-1\right]\right\}.$$

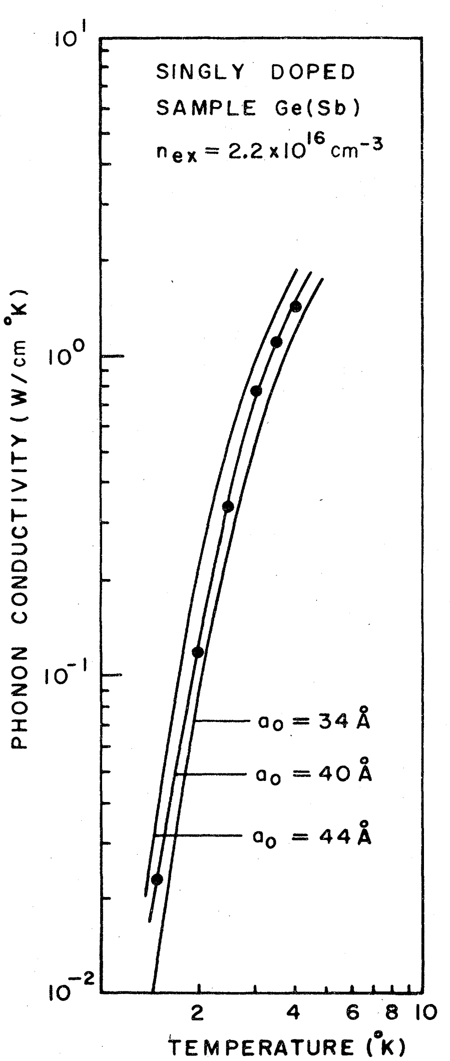


FIG. 1. Variations of phonon conductivity with temperature at different values of effective Bohr radius a_0 for the sample Ge(Sb) (doped with antimony, $n_{ex}=2.2\times10^{16}$ cm^{-3}). Experimental points are shown by filled circles. Theoretical curves are shown by solid lines.

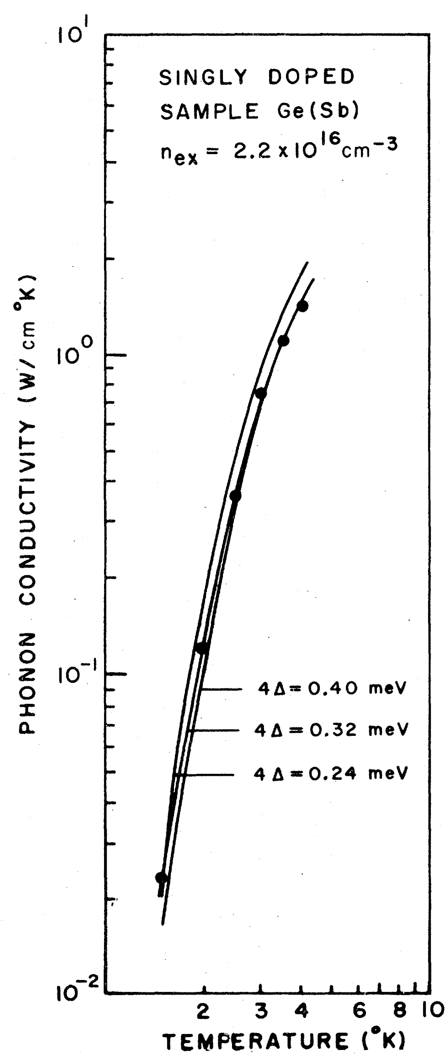


FIG. 2. Variations of phonon conductivity with temperature at different values of chemical shift 4Δ for the sample Ge(Sb) (doped with antimony, $n_{ex}=2.2\times10^{16}$ cm^{-3}). Experimental points are shown by filled circles. Theoretical curves are shown by solid lines.

Here k_B is the Boltzmann constant, j is a polarization index, v_j is the phonon velocity, $x=\hbar\omega/k_BT$, ω is the phonon frequency, q is the phonon wave vector, and $\tau(q,j)$ is the effective relaxation time, which is given by $\tau^{-1}(q,j)=\sum_i \tau_i^{-1}(q,j)$. Further, v_j/L $(=\tau_B^{-1})$ is the relaxation rate due to boundary scattering of phonons, $A(k_B/\hbar)^4x^4T^4$ $(=\tau_{pt}^{-1})$ is the relaxation rate due to point-defect scattering of phonons, $(B_1+B_2)(k_B/\hbar)^2x^2T^5$ $(=\tau_{ph\text{-}ph}^{-1})$ is the relaxation rate due to phonon-phonon scattering, $\tau_{el}^{-1}(q,j)$ is the relaxation rate due to elastic scattering of phonons both from the triplet as well as the singlet states, $\tau_1^{-1}(q,j)$ is the relaxation rate due to inelastic scattering of phonons from the triplet state, and $\tau_2^{-1}(q,j)$ is the relaxation rate due to thermally assisted phonon absorption processes for $\omega_{qj} < 4\Delta/\hbar$ and inelastic scattering by electrons in the singlet state for $\omega_{qj} > 4\Delta/\hbar$. Again ρ is the density of the crystal and Ξ_u is the shear deformation potential. The cutoff factor $f^2(\omega/v_j)$ is given by

$$f^2\left(\frac{\omega}{v_j}\right)=\left[1+\left(\frac{a_0k_B}{2v_j\hbar}\right)^2x^2T^2\right]^{-4},$$

where a_0 is the donor-electron radius. The level-

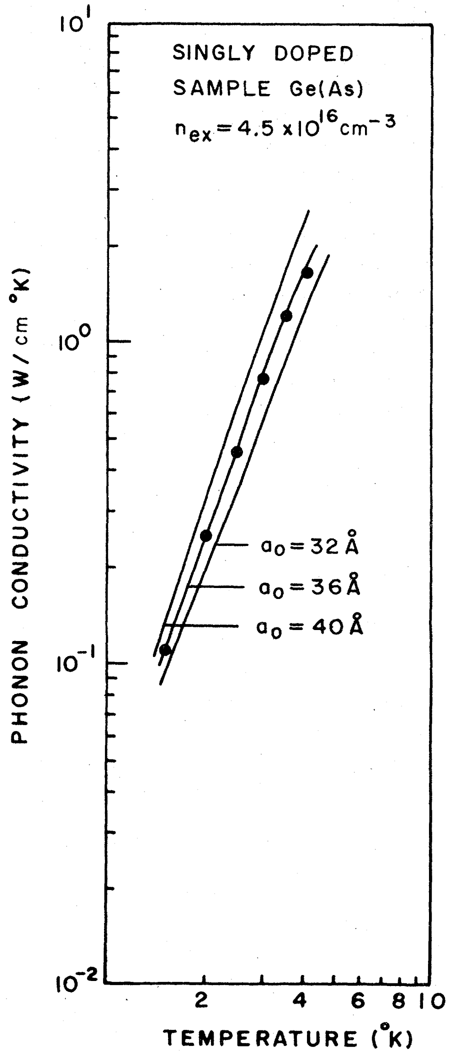


FIG. 3. Variations of phonon conductivity with temperature at different values of effective Bohr radius a_0 for the sample Ge(As) (doped with arsenic, $n_{ex}=4.5\times10^{16}$ cm^{-3}). Experimental points are shown by filled circles. Theoretical curves are shown by solid lines.

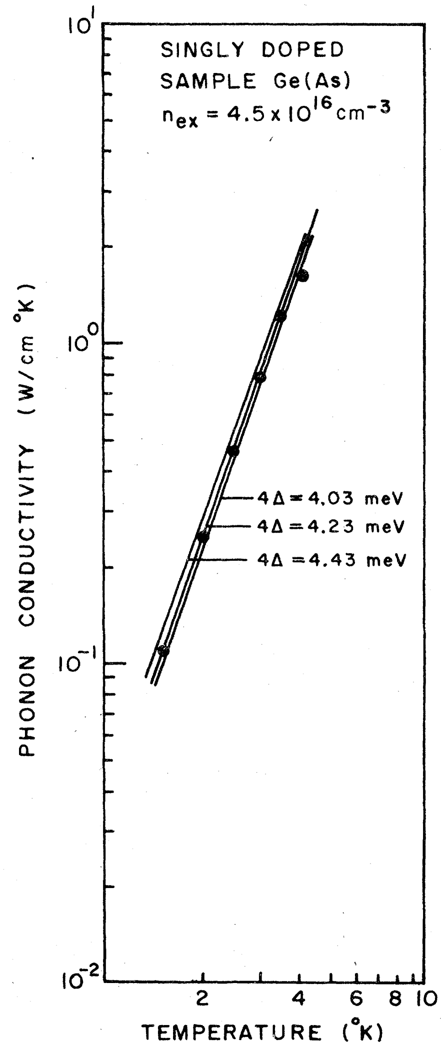


FIG. 4. Variations of phonon conductivity with temperature at different values of chemical shift 4Δ for the sample Ge(As) (doped with arsenic, $n_{ex}=4.5\times10^{16}$ cm^{-3}). Experimental points are shown by the filled circles. Theoretical curves are shown by solid lines.

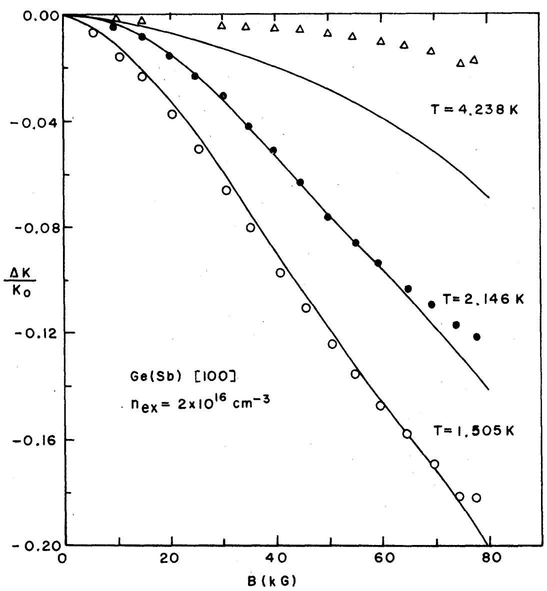


FIG. 5. Plot of $\Delta K/K_0$ with magnetic field at different temperatures for the sample Ge(Sb), $n_{ex} = 2.2 \times 10^{16}$ cm^{-3} with $\vec{B} \parallel [100]$. Experimental results are shown by points and theoretical results by solid lines.

width parameter Γ is given by

$$\Gamma = \Gamma_S + \Gamma_T = \frac{1}{15\pi\rho}\left(\frac{\Xi_u}{3}\right)^2\left(\frac{4\Delta}{\hbar}\right)^3 \Gamma\left(\frac{4\Delta}{\hbar}\right) \times\left(1 + \frac{4}{\exp(4\Delta/k_B T) - 1}\right),$$

where Γ_S and Γ_T are the level widths of the singlet and triplet states. The quantity $F(\omega)$ is given by

$$F(\omega) = \left[\frac{1}{v_1^5} f^2\left(\frac{\omega}{v_1}\right) + \frac{3}{2}\,\frac{1}{v_2^5} f^2\left(\frac{\omega}{v_2}\right)\right].$$

III. RESULTS AND DISCUSSION

First, we show how the theoretical values of the phonon conductivity are changed in the absence of a magnetic field for the two samples when a_0 and 4Δ are varied around the optimum values which give the best fit between theory and experiment. The results of the calculation are shown in Figs. 1–4.

The magnetic field data are shown in Figs. 5 and 6 as $\Delta K/K_0$ vs B (kG) at three different temperatures in the range 1.3 to 4.4°K. Here $\Delta K = K - K_0$, where K is the phonon conductivity in the presence of magnetic field and K_0 is the same in the absence of magnetic field. The adjusted values of a and 4Δ for different values of the magnetic field, which give the best agreement between theory and experiment, are shown as dashed lines in Fig. 7. For magnetic fields greater than 80 kG the curve showing the adjusted values is extrapolated for the sake of comparison with theory. Our adjusted values of a_0 and 4Δ correspond to the experimental values for fields B along the [100] direction. These values are compared with Halbo's calculated values of $4\Delta/4\Delta_0$ and a/a_0 for fields along the [100] direc-

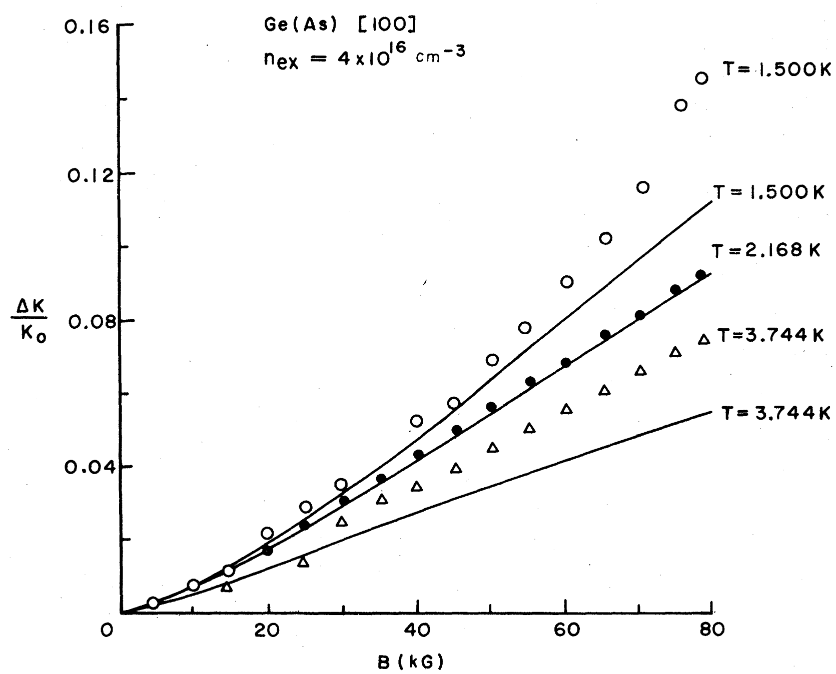
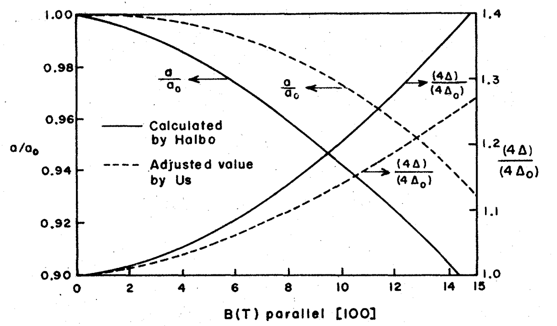


FIG. 6. Plot of $\Delta K/K_0$ for magnetic field at different temperatures for sample Ge(As), $n_{ex} = 4.5 \times 10^{16}$ cm^{-3} with $\vec{B} \parallel [100]$. Experimental results are shown by points and theoretical results by solid lines.



The magnetic field dependence of the effective Bohr radius a_0 and the chemical shift $4\Delta_0$ in singly doped semiconductors.

FIG. 7. Plot of $4\Delta/4\Delta_0$ and a/a_0 vs magnetic field parallel to the ⟨100⟩ direction. Solid lines represent the results of Halbo calculated on the basis of the variational technique. Broken lines are the values adjusted by us for best fit between theory and experiment.

tion.[6] His results are given as solid lines in Fig. 7. The values of the various parameters used for our calculations are given in Table I.

It may be observed from Fig. 7 that in both cases the applied magnetic field causes a shrinkage in the donor-electron radius a_0 and an increase in the value of 4Δ. According to the present calculations, the conductivity always decreases when a_0 is decreased. However, for the variations in 4Δ, the effects on the phonon conductivity of Sb-doped and As-doped Ge are opposite to each other. In Sb-doped Ge, the increase in 4Δ causes a decrease in K, whereas in As-doped Ge the opposite effect is observed. Thus in Sb-doped Ge, the effects of an increase in 4Δ and a decrease in a_0 are in the same direction and the combined effect is to decrease the phonon conductivity with the increase in magnetic field. In As-doped Ge, the effect on K due to the increase in 4Δ dominates over that due to the decrease in a_0. The net effect is that the phonon conductivity increases when the magnetic field is

TABLE I. Values of the various parameters used in the evaluation of the phonon conductivity.

$V_1 = 5.37 \times 10^5$ cm/sec	
$V_2 = 3.28 \times 10^5$ cm/sec	
$A = 2.4 \times 10^{-44}$ sec^3	
$B_1 + B_2 = 2.80 \times 10^{-23}$ sec K^{-3}	
Ge(Sb)	Ge(As)
$N_{ex} = 2.2 \times 10^{16}$ cm^{-3}	$N_{ex} = 4.5 \times 10^{16}$ cm^{-3}
$E_u = 19$ eV	$E_u = 16$ eV
$a_0 = 40$ Å $(H=0)$	$a_0 = 36$ Å $(H=0)$
$4\Delta = 0.32$ meV $(H=0)$	$4\Delta = 4.23$ meV $(H=0)$
$L = 0.489$ cm	$L = 0.373$ cm

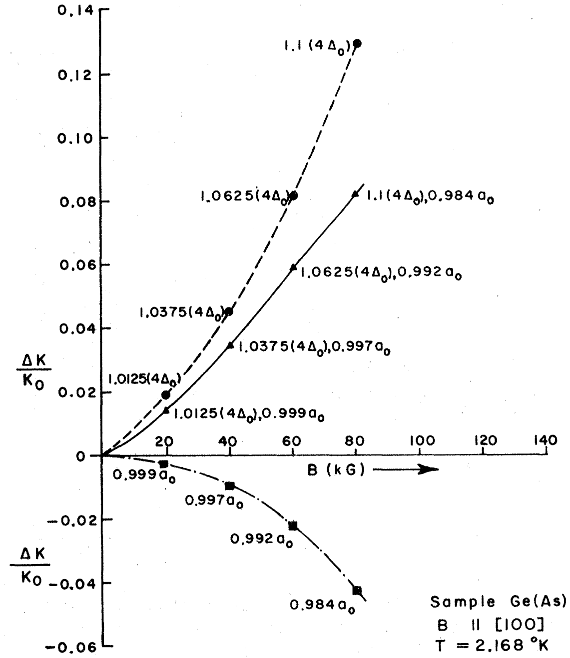


FIG. 8. Plot of $\Delta K/K_0$ vs B for Ge(As). The dashed line shows the effects on $\Delta K/K_0$ when only 4Δ is varied. The dash-dot line shows the variations of $\Delta K/K_0$ when only a_0 is varied. The solid line shows the resultant effect on $\Delta K/K_0$ when both 4Δ and a_0 are varied (the magnetic field affects both a_0 and 4Δ).

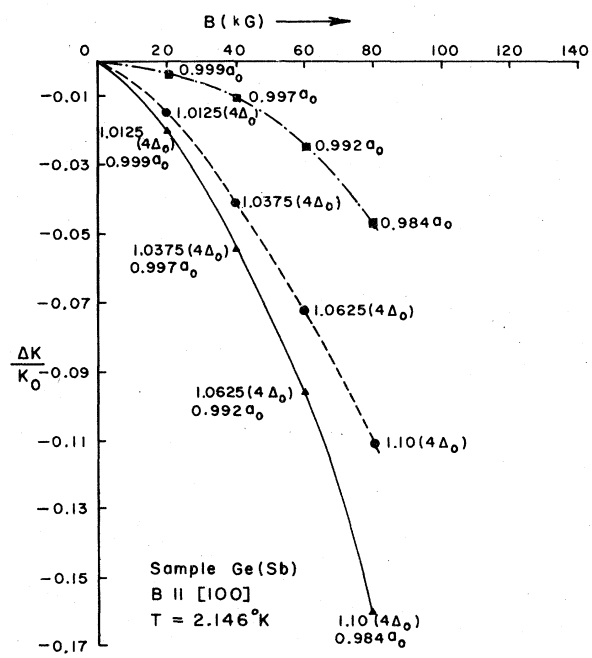


FIG. 9. Plot of $\Delta K/K_0$ vs B for Ge(Sb). The dashed line shows the effect on $\Delta K/K_0$ when only 4Δ is varied. The dash-dot line shows the variations of $\Delta K/K_0$ when only a_0 is varied. The solid line indicates the resultant effect on $\Delta K/K_0$ when both 4Δ and a_0 are varied (the magnetic field affects both a_0 and 4Δ).

increased.

The above discussion can be appreciated better with the help of Figs. 8 and 9, where dashed lines show the variation in phonon conductivity due to increase in the values of 4Δ and dot-dashed lines indicate the corresponding variation with the decrease in the value of a_0. The resultant variations in the values of the phonon conductivity K are shown by the solid lines which indicate opposite effects for Sb- and As-doped Ge.

The magnetic field dependence of P-doped Ge samples oriented in [100] directions is similar to that of As-doped Ge and the present variations of 4Δ and a_0 can also explain the magnetic field results of P-doped Ge. Thus the present curves of $4\Delta/4\Delta_0$ and a/a_0 vs H applied along [100] direction are the universal curves for lightly doped n-type Ge such as Sb-, As-, and P-doped Ge.

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