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THE EFFECT OF NONMETAL-METAL TRANSITION DUE TO DOPING ON LATTICE THERMAL CONDUCTIVITY: APPLICATION TO Ge-DOPED InSb

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Abstract.- In this work we explain the phonon thermal conductivity results of Ge-doped InSb from 2 to 50 K for impurity concentrations $7.2 \times 10^{17}$ and $5.0 \times 10^{17}$ cm$^{-3}$. Since these lie in the intermediate concentration region of the metal-nonmetal transition the theory of scattering of phonon by holes in the mixed state, i.e. both in the localised non-metallic and in the metallic state is used. The hole concentrations in the non-metallic and metallic regions are calculated for each sample by using Mikoshiba's inhomogeneity model, the theory of both bound hole-phonon and free hole phonon scattering are applied to explain the results. The value of density-of-states effective mass are kept constant ($=0.23$) with the variation in temperature. The value of the dilatation and shear deformation potential constants obtained from our calculations are in good agreement with previously determined values. The effect of impurity scattering due to doped impurities along with isotope scattering is also taken into account.

It is reported that in the intermediate concentration range, the mixed hole-phonon scattering must be included to explain the temperature dependence of thermal conductivity of Ge-doped InSb.

Introduction. - The phonon thermal conductivity of p-InSb doped with Ge, has been studied experimentally [1,2] for acceptor hole concentrations from $2.7 \times 10^{14}$ to $6 \times 10^{18}$ cm$^{-3}$. In the low concentration region well below the critical concentration for nonmetal-metal transition ($N_c$) the holes are bound to the impurity atoms and in the high impurity concentration region, they are free in valence band. In the intermediate doping concentration near $N_c$, the holes exist in a mixed state. Using Mikoshiba's "inhomogeneity model", the acceptor hole concentration in both non-metallic and metallic region can be calculated. In the present work we have chosen two samples of p-InSb with $N=7.2 \times 10^{17}$ and $5 \times 10^{17}$ cm$^{-3}$. Using Mott's expression the critical concentration for metal-nonmetal transition ($N_c$) can be given as $N_c=(\frac{\pi^2}{3}a^*)^3$ where $a^*$ is the effective Bohr radius of the
impurity and the concentration at which Fermi level merges with valence band is $N_{vb} = \frac{1}{4\pi}(a^*)^{-3}$. Using $a^* = 38^9\text{Å}$, the values $N_c$ and $N_{vb}$ are calculated to be $2.84\times10^{17}$ and $1.45\times10^{18}$ cm$^{-3}$ for p-InSb. Using Mikoshiba's inhomogeneity model the hole concentrations in nonmetallic and metallic regions can be calculated as $N_n = N \exp\left(-\frac{4}{3}\frac{\pi r_c^3}{N_{vb}}\right)$ and $N_m = (N-N_n)$ where $r_c = \left(\frac{144\pi^2}{N_{vb}}\right)^{1/3} a^*$. For the sample of p-InSb with $N = 7.2\times10^{17}$ cm$^{-3}$ the values of $N_n = 0.64\times10^{17}$ and $N_m = 6.55\times10^{17}$ cm$^{-3}$ and for the sample with $N = 5\times10^{17}$ cm$^{-3}$, $N_n = 0.936\times10^{17}$ and $N_m = 4.06\times10^{17}$ cm$^{-3}$. Using the relaxation rate of bound hole-phonon scattering, for the holes in nonmetallic region and the relaxation rate for free hole phonon scattering for the holes in metallic region, the phonon conductivity values of these two samples in the intermediate doping concentration are explained well between 2 and 50 K.

**Theory.**— The relaxation rate for the bound hole-phonon scattering is given as

$$\left(\frac{1}{\tau_{ep}}\right)_{\text{bound}} = \frac{N_n \omega^2 (2/3 D_u^a)^4 f(q) 20D^4 + 120D^2 + 60}{40\pi \left(\frac{2\pi}{3} \rho \right)^{3/2}}$$

where $f(q) = (1+1/4 a^2 q^2)^{-2}$ and $D = D_u^a/D_u^d$.

$D_u^a$ and $D_u^d$ are the shear deformation potentials for the strains along [001] and [111] directions, $q$ is the phonon wave vector, $v$ is the average phonon velocity and $\rho$ is the density of the crystal.

The acceptor holes in the metallic region can be considered to be free in the valence band and the relaxation rate for the scattering of phonons by free holes for $q \leq 2k_F$ is given as

$$\left(\frac{1}{\tau_{ep}}\right)_{q \leq 2k_F} = \frac{m^* C^2 k_B T \gamma_{1l}^2}{27 \hbar^4 \rho v} \ln \left(\frac{1+\exp\left(\frac{\eta^*-N/T-Px^2}{2}\right)}{1+\exp\left(\frac{\eta^*-N/T-Px^2}{2}\right)}\right)$$

where $N = m^* v^2/2k_B$; $P = k_B/2m^* v^2$ and $\eta^* = \frac{N^2 \hbar^2 (3N_m/N)^2}{2m^* k_B T}$.

$m^*$ is the density of -states effective mass and C is the dilatation deformation potential. For phonon wave vector $q > 2k_F$, the relaxation rate for the scattering of phonons by free holes is given as

$$\left(\frac{1}{\tau_{ep}}\right)_{q > 2k_F} = \frac{185 m^2 C^2 N_m \gamma_{1l}^2}{\hbar^3 q^5 a^* P}$$

The phonon thermal conductivity can be calculated using these expressions by the method described elsewhere [3].
Results and Discussion.— By considering the realistic hole-phonon scattering relaxation rates for the doped samples of p-InSb in the intermediate concentration region, the phonon conductivity values are explained satisfactorily between 2 and 50 K as shown in the figure. The theoretical analysis of hole phonon scattering establishes the existence of holes in a mixed state i.e. both in bound and free impurity states in the region of present interest. The values of shear deformation potentials determined by our theoretical analysis are $D^a_u = 2.8$ eV and $D^s_u = 4.2$ eV; which are in agreement with experimental values. The dilatation deformation potential constants are 1.4 eV and 1.3 eV, for the two samples with $N = 7.2 \times 10^{17}$ and $5 \times 10^{17}$ cm$^{-3}$. The scattering due to doped impurities is also considered in addition to isotope scattering in the calculation for point defect scattering parameter. The values of the parameters are given in the Table.

Table.— Parameters used in the calculation

\[
\begin{align*}
  a^* &= 38 \AA, \quad m^*/m = 0.23, \quad v = 2.3 \times 10^5 \text{ cm s}^{-1} \\
  C_B^{-1} &= 1.6 \times 10^6 \text{ s}^{-1}, \quad \rho = 5.76 \text{ gm cm}^{-3} \\
  A &= 4.36 \times 10^{-44} \text{ s}^3, \quad B = 8.7 \times 10^{-23} \text{ s K}^{-3}
\end{align*}
\]

Figure.— Thermal conductivity of p-InSb samples as a function of Temperature.

References