PROC. 15TH INT. CONF. PHYSICS OF SEMICONDUCTORS, KYOTO, 1980
J. PHYS. SOC. JAPAN 49 (1980) SUPPL. A p. 383–386

THEORY OF RESISTENCE AND HALL MAXIMA IN Sb-DOPED Ge IN THE METALLIC RANGE

Tetsuro Saso and Tadao Kasuya†

Max-Planck-Institut für Festkörperforschung
Stuttgart, West Germany
†Department of Physics, Faculty of Science
Tohoku University, Sendai, 980 Japan

The transport properties of heavily doped semiconductors in the metallic concentration range are investigated by the degenerate electron gas model. Especially, the screening of impurities and the scattering of electrons by them are studied in detail by the Kohn-Sham method. The characteristic maxima in the temperature dependence of resistivity and Hall coefficient of Sb-doped Ge, which has been so far attributed to the existence of impurity band, are naturally explained by the present model.

I. Introduction

Resistivity of heavily doped semiconductors shows an activation type temperature dependence with activation energy ε_1 and ε_3 in the low concentration range, and Hall coefficient shows a maximum [1]. These have been interpreted by the so-called "two band model" in which an impurity band exists below the conduction band and electric conduction can occur in this impurity band at low temperatures. In the high concentration range, the temperature dependence is weak and resistivity and Hall coefficient go to constant values at lowest temperatures. Therefore, the high concentration range is sometimes called as the metallic range. But the activation energy ε_1 and the maxima in Hall coefficient seem to persist even in this range, although the maxima are rather smaller than in the low concentration range. These characters have been so far attributed to the existence of impurity band even in this high concentration range [2]. But experiments on electronic specific heat [3], piezoresistance [4], and de Haas-Shbunikov oscillation [5] seem to be well explained by the degenerate electron gas model without impurity band. Furthermore the detailed experiment on the temperature dependence of resistivity of Sb-doped Ge by Sasaki, et al. [6] shows the characteristic maxima around $T_{max} \sim 0.7 T_F$, where T_F denotes the Fermi temperature obtained by assuming a rigid conduction band. These maxima disappear under the unixial saturation-stress in ⟨111⟩ direction which forces all electrons into a single valley. These experiments can not be explained by the simple two band model, but rather seem to suggest that the degenerate electron gas model might work well. For, in the present case, a large temperature dependence should be expected due to the small Fermi temperature ($\lesssim$100K). Thus in the present report we investigate the transport properties of heavily doped semiconductors, especially of Sb-doped Ge as an example, by the degenerate electron gas model without impurity band.

II. Method of Calculation

By using the Boltzmann equation and the variational method,

longitudinal and transverse conductivities are expressed in the single valley case as $\sigma_{//}=n_1e^2\langle\tau_{//}\rangle/m_{//}$ and $\sigma_{\perp}=n_1e^2\langle\tau_{\perp}\rangle/m_{\perp}$, where n_1 is the number of electrons in a single valley and $\langle\tau_\alpha\rangle(\alpha=//,\perp)$ the thermal average of the electron relaxation time. In the unstressed case with ν valleys, conductivity is given by $\sigma=(\nu/3)(\sigma_{//}+2\sigma_{\perp})$ and Hall coefficient by

$$R_H = \frac{3}{n_e ec}\left(\frac{2\langle\tau_{//}\tau_{\perp}\rangle}{m_{//}m_{\perp}} + \frac{\langle\tau_{\perp}^2\rangle}{m_{\perp}^2}\right)/\left(\frac{\langle\tau_{//}\rangle}{m_{//}} + \frac{2\langle\tau_{\perp}\rangle}{m_{\perp}}\right)^2 , \qquad (1)$$

where n_e is the total number of electrons. The inverse relaxation time is assumed to be given by the simple sum of the contributions from the impurity scattering and the phonon scattering as $1/\tau_\alpha(\varepsilon)=1/\tau_\alpha^{imp}(\varepsilon)+1/\tau_\alpha^{ph}(\varepsilon)$, and the latter is assumed to be given by the sum of the contributions from the acoustic and the optical phonon scattering. $1/\tau_\alpha^{imp}$ is calculated by

$$\frac{1}{\tau_\alpha^{imp}(\varepsilon)} = \left\langle \sum_{\mathbf{k}'} \left(1 - \frac{v_{\mathbf{k}'\alpha}}{v_{\mathbf{k}\alpha}}\right) S(\mathbf{k},\mathbf{k}') \right\rangle , \qquad (2)$$

where $\langle\ldots\rangle$ means the average on the direction of $\mathbf{k}$, $v_{\mathbf{k}}$ the velocity and $S(\mathbf{k},\mathbf{k}')$ the transition probability from $\mathbf{k}$ to $\mathbf{k}'$. In the 1st Born approximation,

$$S(\mathbf{k},\mathbf{k}') = \frac{2\pi N_{imp}}{\hbar}\left(\frac{4\pi e^2}{K}\right)\frac{\delta(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}'})}{[(\mathbf{k}-\mathbf{k}')^2+q_{TF}^2(T)\tilde{F}(\mathbf{K}-\mathbf{k}')]^2} , \qquad (3)$$

where we used the random phase approximation(RPA) for impurity screening, and N_{imp} denotes the number of impurities (which we assume to be equal to n_e), κ the dielectric constant, $q_{TF}(T)$ the Thomas-Fermi screening parameter at finite temperatures and $\tilde{F}(\mathbf{k}-\mathbf{k}')$ is given by the sum of the contribution from ν valleys

$$\tilde{F}(\mathbf{q}) = \frac{1}{\nu}\sum_{i=1}^{\nu} F(|\mathbf{q}|/2|\mathbf{k}_F^{(i)}|) \qquad (4)$$

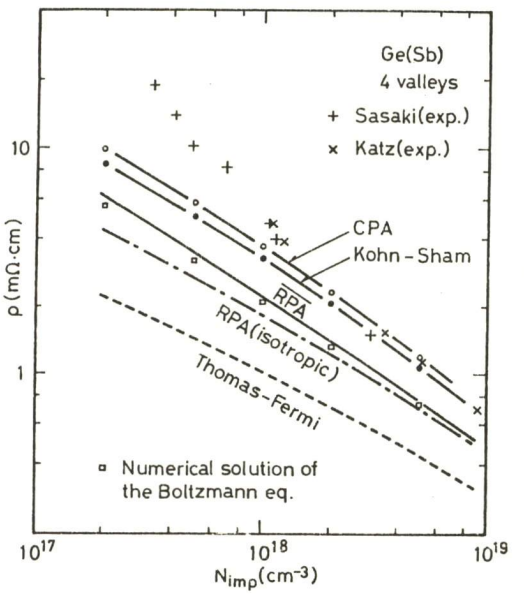

Fig.1

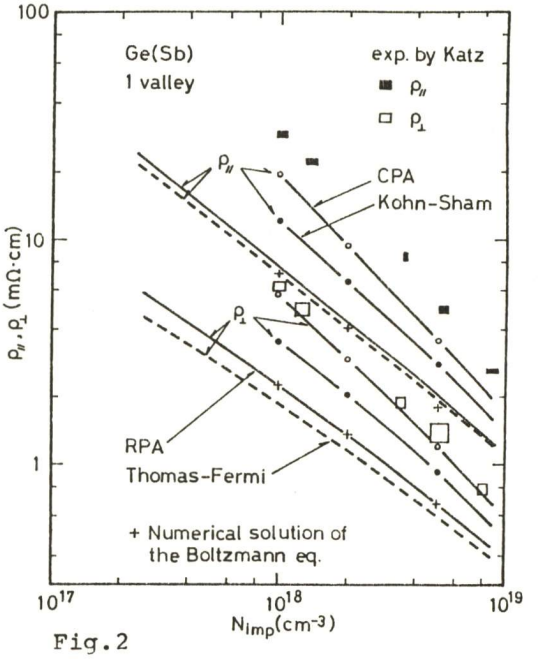

Fig.2

with $k_F^{(i)}$ the Fermi wave vector of i-th valley in the direction of q and F(x) the Lindhard function at finite temperatures. In actual calculation it is sufficient to use its zero temperature form. Furthermore, in the unstressed four valley case, $\tilde{F}(q)$ is averaged over the direction of q. This approximation, as well as the validity of the variational method, was checked by solving the Boltzmann equation directly in a numerical method using the unaveraged $\tilde{F}(q)$. Results at zero temperature, which we will refer to as ρ(RPA(anisotropic)) later, are shown in Figs. 1 and 2 by the full lines which should be compared with those obtained from the exact solution of the Boltzmann equation.

Next, we estimate the effect of nonlinear screening and manybody interaction by the Kohn-Sham method, using the isotropic effective mass $m_d (=(m_{/\!/} m_\perp^2)^{1/3})$. We assume the independent scatterer approximation and neglect the correlation among the positions of impurities. Thus we treat the screening of a single impurity placed in otherwise homogenious electron gas with homogenious positive background, similar to the screening of an impurity in metals. The Schrödinger-like equation with effective potential

$$V(r) = -\frac{e^2}{Kr} + \frac{e^2}{K}\int \frac{n(r')-n_e}{|r-r'|}dr' + V_{xc}[n(r)], \quad n(r) = \sum_n^{occ} |\psi_n(r)|^2 \qquad (5)$$

are solved self-consistently by interaction. In this equation n(r) denotes the charge density of electrons and V_{xc} the exchange-correlation potential, for which we assume that Xα form with α=2/3. After the iteration scheme converges, we can calculate resistivity from the scattering phase shift δ_l(l=0~6). As a result, the resistivity is much enhanced by a factor of 1.5 compared with those obtained with the 1st Born approximation for scattering and RPA for screening (ρ(RPA(isotropic)) in Fig.1). We define the enhancement factor g_{KS} as the ratio of the resistivity obtained by the Kohn-Sham method to those by the RPA and the 1st Born approximation in the isotropic mass approximation. Multiplying this factor to ρ(RPA(anisotropic)), we obtained the values shown in Figs.1 and 2 by the filled circles.

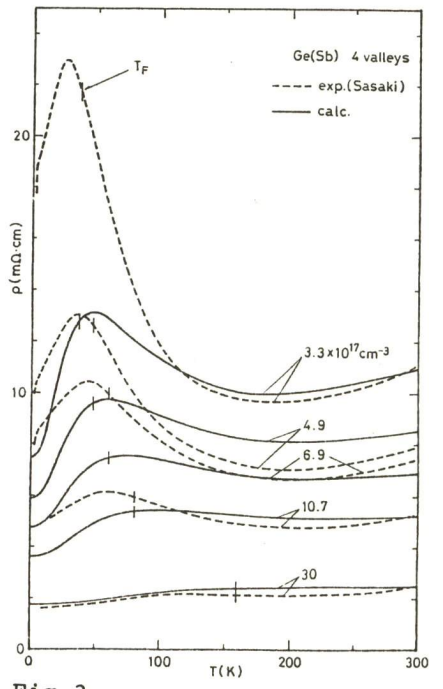

Fig.3

The effect of multiple scattering is calculated by the single site coherent potential approximation (CPA) with δ-function type attractive potential for each impurity with strength V_0 and momentum space cutoff parameter k_c. We choose k_c to be equal to $q_{TF}(T=0)$. V_0 is determined so as to reproduce the values of resistivities shown in Figs.1 and 2 by the filled circles, when the multiple scattering renormalization is omitted in electron self-energy. We define the enhancement factor g_{CPA} as the rato of ρ(CPA) to $g_{KS}\cdot\rho$(RPA(anisotropic)). The results are shown in Figs. 1 and 2 by the open circles. Agreement with experiments is very good except the concentration range lower than $10^{18}cm^{-3}$ in the four valley case.

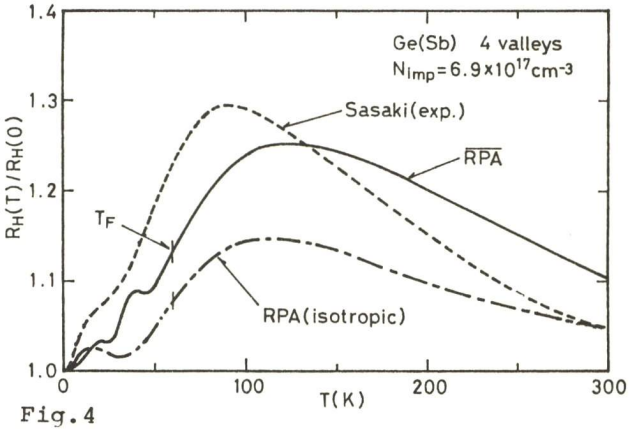

Fig.4

In calculating the temperature dependence of resistivity and Hall coefficient, we take into account the effect of nonlinear screening, etc. by multiplying the factor $g_{KS}g_{CPA}$ to $1/\tau_{\alpha}^{imp}(\varepsilon)$ in eq.(2). Temperature dependence of the enhancement factor is neglected. The result for the unstressed case are shown in Fig.3. The characteristic peaks in the four valley case are well reproduced at the correct positions, though the absolute values are smaller than the experiments in the lower concentrations. The mechanism of the appearance of these peaks is as follows. In the four valley case, the screening length of impurity potential q_{TF}^{-1} is shorter than the electron wave length k_F at T=OK. As temperature increases, the screening length increases but the thermal wave length of electrons decreases. Thus a strong scattering occurs in a resonant fashion at some temperature where the potential range becomes comparable to the thermal wave length of electrons. In the single valley case under uniaxial stress, the screening length is longer than the thermal wave length, thus maxima do not appear in this case.

III. Conclusion

In this report we proposed a detailed calculation of the transport properties of Sb-doped Ge in the metallic concentration range by the degenerate electron gas model without impurity band, including the effect of anisotropic effective mass, the nonlinear screening of impurities, the non-Born scattering, the many-body effect and the multiple scattering by many impurities. Note that the present calculation contains no adjustable parameters. As a result, we could obtain the absolute values of resistivity which agree well with experiments and could reproduce a characteristic maxima in the temperature dependence of resistivity and Hall coefficient, the latter of which has been so far attributed to the existence of impurity band in the high concentration range. There remains some quantitative disagreement with experiments on the values of resistivity in the concentration near N_c. We consider that it is necessary to take into account the effect of impurity clusters in this range. Studies along this line are now under progress.

References

1) H. Fritzsche: J.Chem.Phys.Solids 6 (1958) 69.
2) N.F.Mott: J.Noncrystalline Solids 1 (1968) 1.
3) N.Kobayashi, S.Ikehata, S.Kobayashi and W.Sasaki: Solid State Comm. 24 (1977) 67.
4) M.Nakamura and W.Sasaki: J.Phys.Soc.Jpn. 19 (1964) 236.
5) M.Nakamura: J.Phys.Soc.Jpn. 22 (1967) 830.
6) W.Sasaki: Suppl.Prog.Theor.Phys. 57 (1975) 225; T.Kurosawa, M.Matsui and W.Sasaki: J.Phys.Soc.Jpn.42 (1977) 1622.
7) T.Saso and T.Kasuya: J.Phys.Soc.Jpn. 48 (1980) 1566; 49 (1980) No.2.