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Free Carrier Scattering in Metallic *n*-GaAs in the Presence of Static Lattice Distortions Due to a Partial Chemical Order of Impurities

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Simple electric transport versus $T = 20$–400 K in metallic n-GaAs annealed single crystals with Te impurity concentration $\sim (0.4$–$1.7) \times 10^{19}$ cm^{-3}, which is above the *equilibrium doping limit*, is reported and compared with modern theory of electron mobility in degenerated n-GaAs by Szmyd, Hanna, Majerfeld. An overcome of the equilibrium doping limit in annealed n-GaAs is manifested by a lowered electrical activation of Te donors and by an onset of ≈ 0.1–1 μm regions of local strain in the crystal lattice known from high resolution X-ray studies. These preliminary results of transport show that the electron mobility $\mu(T)$ measured for n-GaAs with local strains is not consistent with predictions of Szmyd et al. model for any degree of compensation assumed. This surprising result indicates that electric transport in materials above the equilibrium doping limit is not well understood assuming the scattering by ionized impurities. The nature of defects responsible for an observed strong reduction of free carrier concentration (here $\approx 80\%$) in annealed heavily doped n-GaAs seems not to be related with electrical compensation. We point here at the possible role of effects of free carrier scattering due to static lattice distortions (local strains) related to a chemical aggregation of impurity atoms. We also notice that transport in metallic n-GaAs with local strains shows features similar to a weak localization $\sigma_{xx} \propto \log T$.

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1. Introduction

Very heavily doped semiconductor materials are important in some regions of electronic devices like highly conductive areas close to ohmic contacts, conducting regions in LEDs and laser diodes transporting carriers to the heterojunction or quantum wells, in channel regions of FET or MOSFET structures or in tunneling devices. In silicon already in late 90-ies the technology of scaling down MOS transistor channel's length, see e.g. Ref. [1], has reached so high dopant concentration that atoms of impurities start to mutually interact chemically in the crystal lattice [2]. This type of interaction may cause a degradation of the devices. It may occur due to such processes as e.g. current-enhanced diffusion of impurities or Fermi level-related impurity aggregation reactions. Often the effects of mutual chemical interaction of impurity atoms and a formation of small aggregates may remain invisible for e.g. plain transmission electron microscopy. Only advanced techniques of structural studies in atomic scale, like STM, could recently identify the pairs of impurity atoms or clusters composed of a few impurity atoms in close lattice sites [3, 4].

In n-GaAs above a certain doping level (concentration of impurities) and related high position of the Fermi level within the band of a degenerated semiconductor there seems to be a tendency of impurity atoms to aggregate by their mutual chemical interaction [5, 6]. Consequently, it may lead to a reduction of free carrier concentration [5–9]. This effect can be called *mutual passivation of impurities*, and it exists above a certain doping level which we call *equilibrium doping limit* [5]. For impurity concentration below this limit the highly doped semiconductor remains stable regarding aging (e.g. by a thermal annealing), as it was noticed for GaAs:Te [5]. The effect of a decrease of free electron concentration in very highly doped n-GaAs was noticed early in single crystals of GaAs doped with all main donor-type elements, like Te, Se [7], Si [8], and S [9]. That time no strong conclusions on the origin of this effect was given, nor probably was possible to reach comparing to today's techniques of structural studies required for identification of responsible defects. One effect which accompanies the formation of small aggregates of impurity atoms (pairs, triples, etc.), still coherent with the host crystal lattice, is a local strain propagating in the lattice surroundings of the aggregate. If aggregates are distributed non-uniformly in the lattice, as it was noticed in the case of GaAs:Te with Te concentration around 1×10^{19} cm^{-3}, showing structural fluctuations with a characteristic length of 0.1–1 μm, the local strain could be measured by high resolution X-ray diffraction [5, 6]. Onset of the local strains accompanied a reduction of free carrier concentration, this reduction could be even as large as e.g. 80% of donors depending on doping level and annealing conditions. In this communication, we report on simple electric transport in n-GaAs with local strain fields.

2. Experimental

We have measured resistivity and Hall effect at T = 20–400 K in heavily doped samples of GaAs:Te which were annealed long time ($\approx$ 200 h) at temperatures 700–800 ℃ resulting in fluctuations of local strain with a characteristic size of 0.1–1 μm and which have free electron concentration reduced by this annealing at $\approx$ 80%, see Table. The details of annealing and the studies by X-rays were briefly described in Refs. [5, 6]. Samples A, B and C contain degenerated free electron gas, having the Fermi level high in the conduction bands, at about 110–120 meV for samples A and B, and about 270 meV for sample C above the bottom of Γ band. The Fermi level calculations above take into account band nonparabolicity and the presence of conduction band minima L and X higher than Γ [10]. For the most interesting case here of sample B, having the free electron concentration much reduced comparing to Te impurity concentration, only one band is occupied around Γ minimum, since the Fermi level is below L and X minima [10], the same being valid for sample A. This simplifies the calculation of mobility, and the one-band model of Szmid, Hanna and Majerfeld [11] (SHM) may be applied. In sample C, having the highest free electron concentration studied here, the concentration of electrons in L band is estimated at about 4×10^{18} cm^{-3} comparing to 1.3×10^{19} cm^{-3} in Γ band, so the contribution to transport in L band remains still small in relation to Γ band, due to about 9 times heavier electrons in L band.

TABLE

Samples of single crystalline GaAs:Te used in these studies. Samples A and C show an almost complete electrical activation of Te donor impurities, n = [Te], where n and [Te] designates the concentration of free electrons and Te impurity atoms, respectively. The free electron concentration n in sample B was lowered by annealing at T = 760 ℃ during 200 h. Sample C was annealed at 1200 ℃ to recover close to complete electrical activation of donor impurities, n = [Te]. Sample A is thermally stable, i.e. carrier concentration is not sensitive to annealing at high temperatures, which in the case of GaAs:Te occurs for Te concentration below equilibrium doping limit at about 4×10^{18} cm^{-3} [5, 6].

Sample	Te concentration	Hall concentration, 300 K
A, #B43RT1	4×10^{18} cm^{-3}	3.8×10^{18} cm^{-3}
B, #B42JA2T1	1.7×10^{19} cm^{-3}	3.5×10^{18} cm^{-3}
C, #B42J2T2	1.7×10^{19} cm^{-3}	1.6×10^{19} cm^{-3}

3. Results and discussion

Since the samples A and B are strongly degenerated, one could expect the electron drift mobility at low temperatures to be independent of temperature (metallic case, dominance of ionized impurity scattering assumed). Within the relaxation time approximation, an averaging of relaxation time over electron energy $\langle\tau\rangle$ yields the relaxation time at the Fermi level $\tau(E_{\rm F})$ and $\mu = e\langle\tau\rangle/m^* = e\tau(E_{\rm F})/m^*$, where m^* is effective mass in the Γ minimum. This type of behavior is well visible in Fig. 1 for temperatures below $\approx$ 200 K for samples A, and also for sample C having higher concentration of free electron gas. The difference between the measured Hall mobility and calculated drift mobility (according to SHM model [11]) due to the Hall factor $r_{\rm H} = \langle\tau^2\rangle/\langle\tau\rangle^2$ should be insignificant for a degenerated case when $r_{\rm H} = 1$. It may be noticed that SHM model of mobility relatively well describes the measured values. The model assumes no adjustable parameters other than the acceptor to donor ratio $N_{\rm A}/N_{\rm D}$, it also includes the conduction band description (nonparabolicity, effective mass) within $k\cdot p$ approximation.

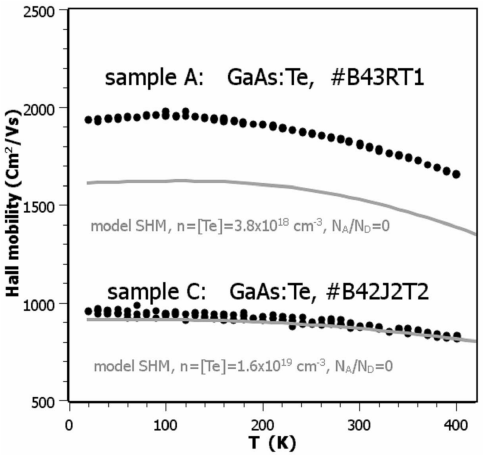

Fig. 1. Measured Hall mobility and calculated electron drift mobility for GaAs:Te samples A and C from Table. For calculations within SHM [11] model the compensation ratio $N_{\rm A}/N_{\rm D}$ = 0 was assumed. It is seen that for lower doped sample A the SHM model underestimates the mobility. Above $\approx$ 200 K the scattering due to phonons is visible.

The interesting case of sample B is shown in Fig. 2. Contrary to the results of measurements for sample A, having similar free electron concentration and Fermi level position as sample B, in case of sample B the SHM model does not describe well the measured mobility. The mobility of sample B drops down going to low temperatures much more rapidly than SHM model can predict for any ratio of electrical compensation $N_{\rm A}/N_{\rm D}$ assumed. In Fig. 2 the predictions of SHM model are shown for several values of compensation ratios. This experimental result seems highly surprising in a degenerated case, where the mobility should be nearly constant versus temperature, as it was in the case of samples A and C. Although the exact mechanism of scattering which depends on temperature so strongly in a degenerated limit is not known in the present, we may suppose that it is related to the local strain field present in the sample doped above the equilib-

rium doping limit and subsequently annealed to decrease the free electron concentration. This local strain fields introduce local perturbations of the crystal lattice periodicity. Consequently, the Bloch waves might be scattered by these perturbations in a similar manner as it is treated in the case of scattering by acoustic phonons. Increasing temperature, the effect of local strain on the effective scattering of electrons seems to be decreased e.g. due to an influence of phonons. In other words, it seems that the description of an effect of scattering at low temperatures in sample B should not be solely from averaging the relaxation time over electron energy, but also should assume an interaction of electrons with the lattice local distortions. As it was measured using high resolution X-ray diffraction [5, 6], the essential difference between samples A (doped below the equilibrium doping limit) and B (doped above the doping limit and relaxed in the sense of lattice supersaturation with impurities) is related to local structural fluctuations present in sample B. These local fluctuations were identified as local strain fields [5, 6].

Yet another observation confirming that the relaxation time responsible for lowered mobility of sample B at low temperatures is not solely an electron effect is given by the Hall concentration measured versus temperature $T = 20$–400 K. It was observed that the Hall electron concentration in sample B increased by about 15 percent decreasing the temperature from 400 K to 20 K. An increase of the Hall concentration in a degenerated case indicates that the Hall factor r_{H} increases at low temperatures by the same 15 percent. This should not occur in degenerated material if the relaxation time were dependent only on the electron energy, as in case of e.g. ionized impurity scattering. This again indicates that lattice disorder plays an important role.

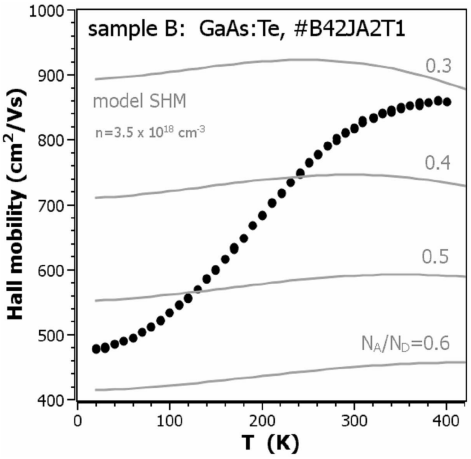

Fig. 2. Measured Hall mobility and calculated electron drift mobility for sample B. For none of compensation ratio $N_{\mathrm{A}}/N_{\mathrm{D}}$ assumed calculations within SHM [11] model were able to properly describe the measured mobility for degenerated electron gas in GaAs:Te for a case of electron concentration reduced by annealing to values equivalent to the equilibrium doping limit.

One more consequence of the above results is a conclusion that *not* an electrical compensation is responsible for $\approx 80\%$ drop of free carrier concentration following sample annealing at $\approx 700\,^{\circ}\mathrm{C}$. Effects leading to this decrease are not purely electronic. This reduction seems to be a complicated process involving the structural changes in the crystal lattice.

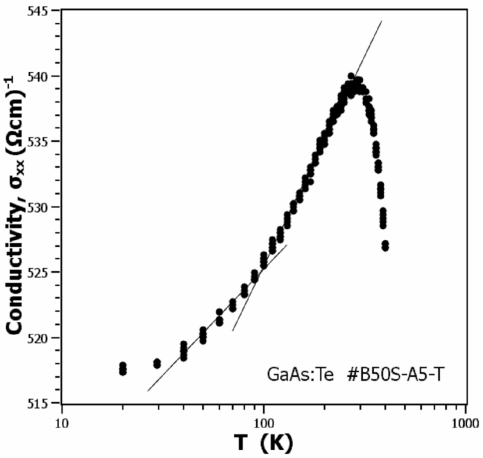

Fig. 3. Plot of conductivity σ_{xx} vs. $\log T$ for GaAs:Te sample with Te concentration 1×10^{19} cm^{-3} and free electron concentration reduced to 4×10^{18} cm^{-3} by annealing. Linear dependence of conductivity versus $\log T$ in temperature ranges 40–100 K and 100–250 K may suggest weak localization effects in transport.

Finally, in Fig. 3 we plot the conductivity versus $\log T$ for "chemically relaxed" sample GaAs:Te with Te concentration $\approx 1 \times 10^{19}$ cm^{-3} (sample not shown in Table). This type of plots is used to recognize features of the weak localization [12], which usually is ascribed to quantum interferences of the Bloch waves in a conductor. Figure 3 shows that in case of chemically relaxed GaAs:Te doped above the equilibrium doping limit, effects similar to the weak localization are observed. It is far from clear now how quantum interferences are enhanced in this type of disordered material with local strain fields.

4. Conclusions

We have shown that electric transport in the single crystal of GaAs:Te doped above the equilibrium doping limit and relaxed in the sense of supersaturation of lattice with impurities is a complicated phenomenon, involving the lattice effects in addition to electronic ones. Lattice disorder, interpreted as local strain fields (local distortions), seems to play a role in free carrier scattering.

Acknowledgments

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