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# $C\!-\!2\!-\!1$ theory for electron mobility in ternary mixed semiconductors

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I. <u>Introduction</u> Electronic transport properties of elemental and binary-compound semiconductors such as Ge, Si, InSb, and GaAs have been comprehensively investigated in theoretical and experimental works. Theory for transport properties of ternary mixed semicondcutors has been reported by several papers<sup>1) - 6)</sup> in which different approaches were taken. Most of theory were applied mainly to  $In_{1-x}Ga_{x}As$ . On the other hand, experimental data have been widely spread. Thus, further basic study is required to see what the transport properties of ternary mixed semiconductors might be. The difficulty in this study is caused by unknown scattering potentials due to the disorder occupation of composite atoms in mixed semiconductors.

In the past studies the disorder scattering potential was considered to be the difference in band gap<sup>1)</sup> or electron affinity<sup>3)</sup> of composite semiconductors, or the potential determined empirically was used<sup>5)</sup>. The band gap or the electron affinity can be considered the properties determined for a bulk material. It is hard to justify that the misoccupation of composite atom due to the disorder causes, near the misoccupation lattice site, the difference in the bulk material properties. In another past study, the deviation in the Coulombic potential at the composition rate of x=0.5 was used as the scattering potential for mixed semiconductors.<sup>6)</sup>

In this paper we propose that the disorder scattering potentials are due to the deviations in the polarization field of Callen's effective charge and in the Coulombic potential calculated at each composition rate of x=x. These deviations can be justified to be caused by the misoccupation of composition atoms in mixed semiconductors. The theory is applied to 14 different mixed semiconductors available from the possible combination of binary III-V compound semiconductors: AlAs, AlSb, GaP, GaAs, GaSb, InP, InAs, and InSb.

II. Theory Taking the consideration of the long-range order parameter R, we have derived the relaxation time  $\tau_d$  for the disorder scattering due to the disorder of the A and B atoms in a mixed semiconductor  $A_{1-x}B_x^{C^{4)}}\tau_d^{-1} = (\sqrt{2}\pi\hbar^4/m^*/\varepsilon) \cdot [(1-R) \times (1-x)n_a(\Delta u_{A\beta}^2 \Delta v_{A\beta}^2 + \Delta u_{B\alpha}^2 \Delta v_{B\alpha}^2)]^{-1}$ . (1)\*

In the theory, the analysis is carried out using the virtual crystal model.<sup>7)</sup> We derive the scattering potential  $\Delta u_p$  caused by the deviation of covalent radius,  $(1/r_i) - (1/r_v)$ . The potential is  $\Delta u_p = (be^2 Z/4\pi\epsilon_0) \cdot |(1/r_i) - (1/r_v)| \cdot exp(-k_s R_{av})$  (2)\*

Cation and anion atoms in a compound semiconductor possess a so-called effective charge which produces polarization. We derive the scattering potential  $\Delta u_c$  due to the polarization deviation,  $(e_1^* - e_v^*)d$ . The potential is  $\Delta u_c = (e_1^* - e_v^*)d/\varepsilon_0\Delta V$  (3)\*

III. <u>Theoretical Results</u> The electron drift mobilities calculated on the basis of only the disorder potentials are shown in Figs. 1 and 2 where complete disorder, R=0, has been assumed. Besides the disorder scattering, the electron transport in a direct conduction band is subjected to the polar optical, the ionized impurity, and the piezoelectric scatterings, whereas the transport in an indirect conduction band is subjected to the intravalley acoustic and the equivalent intervalley scatterings. The electron drift mobilities involving these scatterings are shown in Figs. 3 and 4 where they are calculated for the impurity concentration,  $n=10^{16}$  cm<sup>-3</sup>, and complete disorder, i.e., R=0, is assumed. The electron drift mobilities are also calculated for the mixed semiconductors with perfect order, i.e., R=1, in which the disorder scattering is not involved in the calculation. Theoretical results are shown in Figs. 5 and 6.

Even though the disorder scattering exists in  $InSb_{1-x}As_x$ , the larger mobility in this mixed semiconductor relative to that of InSb could be expected. The electron mobilities of  $In_{1-x}Ga_xAs_x$  and  $InAs_{1-x}P_x$  are very similar when the disorder scattering is not involved as seen in Fig. 5.

\* The detail description of the theoretical process is given at the conference.

The mobility of  $InAs_{1-x}p_x$  is much reduced, due to disorder scattering, relative to that of  $\ln_{1-x}$  Ga As, as seen in Fig. 3, since the difference in the effective charge between InAs and InP is larger than that between InAs and GaAs.

In the mobility variation of the semiconductors alloyed with a direct- and an indirect-band semiconductors, the abrupt decrease is appeared near the band structure transition from the direct

to the indirect band, as seen in Figs. 2, 4, and 6. The composition rate for this transition to occur is x = 0.41 and x = 0.68 in GaAs<sub>1-x</sub>P<sub>x</sub> and In<sub>1-x</sub>Ga<sub>x</sub>P, respectively. This can be attributed to the fact that the effective mass is much heavier in the indirect conduction band as compared with that in the direct conduction band.

The scattering IV. Conclusions potentials have been given by the potential and the polarization deviations caused by the misoccupation of composite atoms. Using these scattering potentials, we have derived the mobility variations with the composition rate of mixed semiconductors. These mobility variations are considered very important in the analysis of microwave and opto-

(cm<sup>2</sup>/v.s)

MOBILITY

DRIFT

ELECTRON

(cm<sup>2</sup>/v.s)

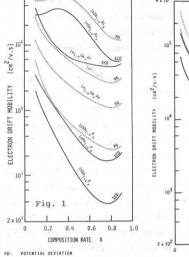
MOBILITY

DRIFT

CTRON

electronic devices fabricating with the mixed semiconductors such as In Ga As and GaAs - P. At the conference, the mobility variations of other 8 mixed semiconductors such as Ga\_In\_\_\_Sb and Ga\_\_Al\_As, the detail description of the theory, and the physical interpretation of the results are presented.

References 1)H.Brooks, Private comm. 2) L. Makowski, et al., J. Phys. Chem. Soilds, 34(1973)487. 3) J.W.Harrison, et al., J. Appl. Phys. 47(1976) 292. 4) A. Sasaki et al., Proc.8th Conf.Solid State Devices(1976)239. 5)T. Nishinaga et al., J. Phys. Soc.Japan, 41 (1976) 1603. 6)F.Ohsaka et al., Japan. J.appl.Phys.15(1976)2371. 7) J.C. Phillips, Bonds and Bands in Semiconductors (Academic Press, New York, 1973)212.



EFFECTIVE CHARGE ( OR POLARIZATION ) DEVIATION

-50-

ECO:

