

# ON A SIMPLIFIED ANALYSIS OF THE CARRIER CONTRIBUTION TO ELASTIC CONSTANTS OF SEMICONDUCTOR SUPERLATTICES

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An attempt is made to present a simplified analysis of the carrier contribution to elastic constants of semiconductor superlattices, taking  $G_{\alpha_1-z}$  Al<sub>x</sub>As<sub>1-x</sub> superlattice as an example. It is found, that the second and third-order elastic constants increase with increasing carrier degeneracy with enhanced numerical values as compared with that of the constituent materials. In addition, we have suggested an experimental method of determining such contributions from degenerate materials having arbitrary dispersion laws.

## I. INTRODUCTION

In recent years, with the advent of MBE, FLL, MOCVD and other fabrication techniques, the realization of semiconductor superlattices (SLS) has been possible [1]. The SL, as originally proposed by Esaki and Tsu [1,2] has found many wide applications in many new device structures, such as avalanche photodiodes [3], photodetectors [4], transistors [5], light-emitters [6], electro-optic modulators [7,8], etc. Nevertheless, it appears from the literature that the carrier contribution to the elastic constants of SLS has yet to be worked out. It is well-known that the carrier contribution to the elastic constants depends on the density-of-states function [9]. Therefore, in SLS, the carrier contribution to the elastic constants will be rather significant due to the property of formation of minibands in such semiconductor heterostructures.

In what follows, we shall present a simplified analysis of the carrier contribution to the second and third-order elastic constants of SLs in section 2.1 of theoretical background. We shall also suggest an experimental method of determining such contributions from degenerate materials having arbitrary carrier dispersion laws in section 2.2. We investigate the doping dependences of the above contributions both from the SL and that of the constituent materials for the purpose of relative comparison taking  $(\text{Ga}_{1-x}\text{Al}_x\text{As})/\text{AlAs}$  SL as an example.

## II. THEORETICAL BACKGROUND

1. In a strained material, only the second and the third-order elastic constants (hereafter referred to as  $C_{44}$  and  $C_{456}$ ) are affected [9]. The carrier contribution to  $C_{44}$  and  $C_{456}$  can, respectively, be written [10] as

$$\Delta C_{44} = \frac{a_0^2}{9} \int_{E'}^{\infty} N(E) \left[ \frac{\partial f_0}{\partial E} \right] dE \quad (1)$$

$$\Delta C_{456} = \frac{a_0^3}{27} \int_{E'}^{\infty} N(E) \left[ \frac{\partial^2 f_0}{\partial E^2} \right] dE \quad (2)$$

where  $a_0$  is the deformation potential constant,  $N(E)$  is the density-of-states function,  $E'$  can be expressed through the equation  $N(E') = 0$  and  $f_0$  is the Fermi-Dirac occupation probability factor. It appears, then that, the evaluations of  $\Delta C_{44}$  and  $\Delta C_{456}$  require an expression of  $N(E)$ , which, in turn is determined by the carrier energy spectrum. In the tight-binding approximation, the electron dispersion law in SL can be expressed [11] as

$$E = \hbar^2(K_x^2 + K_y^2)/2m^* + E_{0s} - E_{1s} \cos(2\pi K_z/K_0) \quad (3)$$

where  $E$  is the total energy of an electron as measured from the the edge of the conduction band of the material with smaller band gap,  $\hbar = h/2\pi$ ,  $h$  is Planck constant,  $m^*$  is the effective electron mass in the bulk of the material constituting the potential wells in the layered structure,  $S$  ( $= 1, 2, 3, \dots$ ) is the miniband index,  $K_0 = 2\pi/d_0$ ,  $d_0$  is the SL period,  $E_{0s}$  and  $E_{1s}$  are the band-center energy and the half-width of the  $S$ -th miniband respectively. The combining (1), (2) and (3) we get

$$\Delta C_{44} = -\frac{m^* a_0^2}{9\hbar^2 d_0} \sum_{s=1}^{s_{\max}} F_{-1}(\eta_s) \quad (4)$$

$$\Delta C_{456} = \frac{m^* a_0^3}{27d_0 K_B T \hbar^2} \sum_{s=1}^{s_{\max}} F_{-2}(\eta_s) \quad (5)$$

where  $\eta_s = (k_B T)^{-1}(E_F - E_{0s})$ ,  $k_B$  is Boltzmann constant,  $T$  is temperature,  $E_F$  is the Fermi energy and  $F_j(\eta_s)$  is the one parameter Fermi-Dirac integral of order  $j$  which can be defined as [12]

$$F_j(\eta_s) = (\Gamma_{j+1})^{-1} \int_0^{\infty} Y^j [1 + \exp(Y - \eta_s)]^{-1} dY; \quad \text{for } j > -1; \quad (6)$$

or for all  $j$ , analytically continued as a complex contour integral around the negative axis:

$$F_j(\eta_s) = A_j \int_{-\infty}^{0^+} [1 + \exp(-Y - \eta_s)]^{-1} Y^j dY. \quad (7)$$

where  $A_j = \Gamma_{-j}/(2\pi\Gamma_{-1})$ .

It appears then that the evaluation of  $\Delta C_{44}$  and  $\Delta C_{456}$  as a function of carrier degeneracy requires an expression of the carrier statistics, which can be expressed as

$$n_0 = \frac{m^* K_B T}{\pi \hbar^2 d_0} \sum_{s=1}^{s_{\max}} F_0(\eta_s) \quad (8)$$

The carrier contribution to the second and third order elastic constants of SL given by (4) and (5) would now be compared to that obtained from the constituting compounds whose energy band structures could be defined by parabolic energy bands for the purpose of simplicity. The expressions of  $\Delta C_{44}$ ,  $\Delta C_{456}$  and  $n_0$  for bulk specimens of the forming materials can, respectively, be written [10] as

$$\Delta C_{44} = -\frac{a_0^2}{9K_B T} N_c F_{-\frac{3}{2}}(\eta) \quad (9)$$

$$\Delta C_{456} = \frac{a_0^3 N_c}{27K_B^2 T^2} F_{-\frac{5}{2}}(\eta) \quad (10)$$

$$n_0 = N_c F_{\frac{3}{2}}(\eta) \quad (11)$$

where  $\eta = E_F/k_B T$  and  $N_c = 2(2m^* \pi k_B T/\hbar^2)^{3/2}$ .

2. Now we consider the materials with arbitrary carrier dispersion law. The thermoelectric power of degenerate materials, having arbitrary carrier energy spectra, in the presence of a classically large magnetic field can be expressed [13] as

$$G = \frac{\pi^2 K_B^2 T}{3e n_0} \left( \frac{\partial n_0}{\partial E_F} \right) \quad (12)$$

Thus combining (1), (2) and (12) we get

$$\Delta C_{44} = -\frac{n_0 e G a_0^2}{3\pi^2 K_B^2 T} \quad (13)$$

$$\Delta C_{456} = \frac{a_0^3 n_0 G^2}{3\pi^4 K_B^3 T} \left[ 1 + (n_0 G^{-1}) \left( \frac{dG}{dn_0} \right) \right] \quad (14)$$

Thus we can experimentally determine  $\Delta C_{44}$  and  $\Delta C_{456}$  for any material by knowing the experimental  $G$  versus  $n_0$  plot of that material.

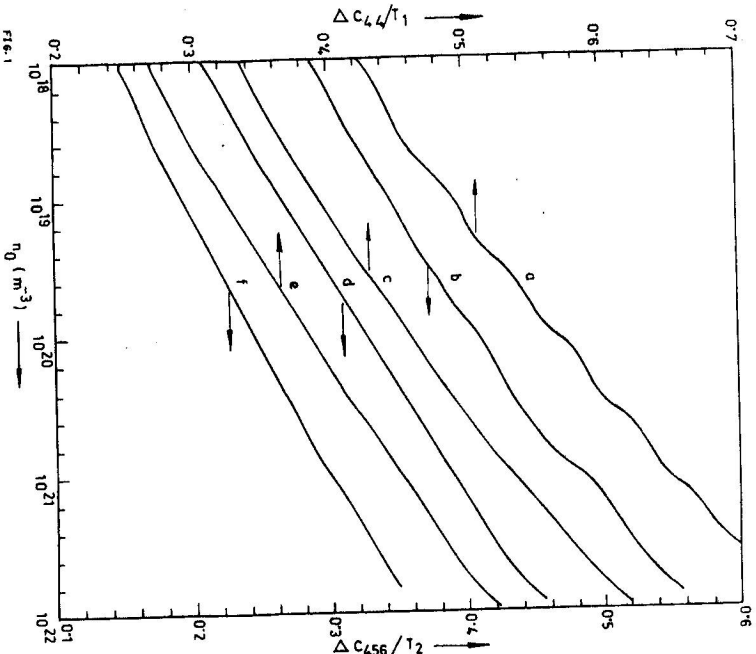


Fig. 1. Plots a and b show the variations of  $\Delta C_{44}/T_1$  and  $\Delta C_{456}/T_2$  for  $\text{Ga}_{1-x}\text{Al}_x\text{As}/\text{GaAs}$  SL as functions of  $n_0$ . Plots c and e exhibit the variations of  $\Delta C_{44}/T_1$  for GaAs and AlAs. Plots d and f exhibit the variations of  $\Delta C_{456}/T_2$  for GaAs and AlAs.

### III. RESULTS AND DISCUSSION

Using (4), (5) and (8) and taking  $\text{Ga}_{1-x}\text{Al}_x\text{As}/\text{AlAs}$  SL having the material constants [14,15]  $m^* = (0.067 + 0.083x)m_0$ ,  $x = 0.2$ ,  $d_0 = 8$  nm,  $E_{01} = 0.05$  eV,  $E_{02} = 0.04$  eV,  $E_{03} = 0.03$  eV and  $T = 4.2$  K, we have plotted in Fig. 1  $\Delta C_{44}/T_1$  ( $T_1 = -n_0 a_0^3 / 9k_B T$ ) and  $\Delta C_{456}/T_2$  ( $T_2 = n_0 a_0^3 / 27(k_B T)^2$ ) as functions of  $n_0$  in which the same dependence has also been plotted considering (9) - (11) for the constituent materials for the purpose of relative comparison. We have considered

the first few minibands, since in an actual SL only the few minibands are being significantly populated at low temperatures where the SL effect becomes prominent.  $\Delta C_{44}$  and  $\Delta C_{456}$  are functions of the Fermi energy, which increases with the increasing electron concentration in an oscillation manner for SL. Therefore  $\Delta C_{44}$  and  $\Delta C_{456}$  will increase in an oscillatory way with increasing  $n_0$ . Since the differentiation of a monotonic increasing function decreases the curvature,  $\Delta C_{456}$  changes almost linearly with  $n_0$ . The numerical values of  $\Delta C_{44}$  and  $\Delta C_{456}$  are greatest for the SL and the least for the constituent materials having parabolic energy bands. Thus the SL structure enhances the carrier contribution to elastic constants.

Our experimental suggestion for the determination of  $\Delta C_{44}$  and  $\Delta C_{456}$  for any degenerate material having arbitrary carrier energy spectrum given by (13) and (14), do not contain any band parameter excluding  $G$ . Only the experimental values of  $G$  for any model as a function of  $n_0$  at a constant temperature will give the experimental values of  $\Delta C_{44}$  and  $\Delta C_{456}$  for that range of carrier concentration for that model. Since the experimental values of  $G$  for the present structure are not known in the literature to the best of our knowledge we can not compare our theoretical formulation with the proposed experiment. The experimental values of  $G$  will provide an experimental check of the  $\Delta C_{44}$  and  $\Delta C_{456}$  and also a technique for probing the band structure in such heterostructures.

We wish to note that in view of the large changes of the elastic constants with  $n_0$ , detailed experimental work on the second- and the third-order elastic constants as functions of carrier degeneracy would be interesting in SLs. It may also be suggested that the experiments on the velocity of sound involving the shear mode as a function of  $n_0$  may exhibit the carrier contribution to the elastic constants of semiconductor heterostructures. Finally it may be noted that the above statements again suggest experimental determinations of  $\Delta C_{44}$  and  $\Delta C_{456}$ , besides the suggested experimental methods of determining them as mentioned above.

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