ISSN 0015—3206
FZKAAA 23 (4) 349 (1991)

LETTER TO THE EDITOR

ON THE ELECTRONIC CONTRIBUTION TO ELASTIC CONSTANTS OF ULTRATHIN FILMS OF p-TYPE Si

KAMAKHYA PRASAD GHATAK

Department of Electronics and Telecommunication Engineering, University of Jadavpur, Calcutta-700032, India

and

BADAL DE

Department of Electrical Engineering, John Brown E and Cinc., 333 Udlow Street, P. O. Box 1422, Connecticut-0690, USA

Received 15 August 1991

UDC 538.975

Original scientific paper

In this paper we have formulated the electronic contribution to the elastic constants in ultrathin films of p-Si by considering the influence of heavy, light and split-off holes, respectively. We have suggested an experimental method of determining the same in degenerate materials having arbitrary dispersion laws. The elastic constants increase with increasing hole concentration in an oscillatory way and decrease with increasing film thickness.

The remarkable development of FLL, MBE, MOCVD and other experimental techniques have generated significant possibilities of fabricating new artificial materials known as quantum cells formed between two planar heterojunctions[1]. Heterostructures based on various materials are currently widely investigated because of the enhancement of carrier mobility[2]. In such structues the electron gas is 2D due to QSE and find extensive applications in quantum well lasers, heterojunction FET's high-speed digital networks and other devices[3]. Though considerable work has already been done, nevertheless the electronic contribution to elastic constants has relatively been less studied[4]. In this paper we shall study the electronic contribution to the eleastic constants in ultrathin films of p-Si by considering the influences of heavy, light and split-off holes, respectively.

In a studied material only the second and the third order elastic constants (hereafter referred to as $\overline{C}_{44}$ and $\overline{C}_{456}$) are affected[4]. The carrier contribution to $\overline{C}_{44}$ and $\overline{C}_{456}$ per-subband can, respectively, be expressed for the present case by extending the method as given elsewhere[4] as

$$\delta(\bar{\Delta}\, C_{44}) = (a_0^2/9d_x) \int N(E) \frac{\partial f_0}{\partial E} \mathrm{d}E \tag{1}$$

and

$$\delta(\bar{\Delta}\, C_{456}) = (a_0^3/27d_x) \int N(E) \frac{\partial^2 f_0}{\partial E^2} \mathrm{d}E \tag{2}$$

where a_0 is the deformation potential constant, d_x is the width of the ultrathin film, $N(E)$ is the density-off-states function, under size quantization per subband, f_0 is the Fermi-Dirac probability factor and E is the total carrier energy as measured from the edge of the valence bands in the absence of quantizating in the vertically downward direction. The energy spectral of the heavy, light and split-off holes in bulk specimens of p-type Si can be written, with the notations of Ref. 5 as

$$E_1 = (A - B)\, k^2 \tag{3}$$

and

$$E_{2,3} = (Bk^2/2) + (Ak^2) - (\Delta/2) \pm \left[B^2 k^4 + \left(\frac{\Delta}{2} + \frac{Bk^2}{2}\right)^2\right]^{1/2}. \tag{4}$$

The total surface hole concentration in ultrathin films of p-type Si is given by

$$p_0 = 2^{-1} [C^{-1} \sum_{n_1=0}^{n_{1max}} (A_1(E_F) + A_2(E_F)) + a_1^{-1} \sum_{n_2=0}^{n_{2max}} (A_3(E_F) +$$

$$+ A_4(E_F)) + (a_1)^{-1} \sum_{n_3=0}^{n_{3max}} (A_5(E_F) + A_6(E_F))] \tag{5}$$

where $A_1(E_F) = (E_F - C(\pi n_1/d_x)^2)$, E_F is the Fermi energy in the present case, $C = (A - B)$,

$$A_j(E_F) = \sum_{r=1}^{S} V_r [A_i(E_F)],$$

j and i are sets of even and odd integers, r is the set of real integers,

$$V_r = 2(k_B T)^{2r} (1 - 2^{1-2r})\, \zeta(2r) \frac{\mathrm{d}^{2r}}{\mathrm{d}E_F^{2r}}, \quad A_3(E_F) = \left[\gamma_+(E_F) - a_1 \left(\frac{n_1 \pi}{d_x}\right)^2\right],$$

$$A_5(E_F) = [\gamma_-(E_F) - a_1(\pi n_3/d_x)^2], \qquad \gamma_\pm(E_F) = [a_2 + a_3 E_F \pm$$

$$\pm \{a_4 E_F^2 + a_5 E_F + a_6\}^{1/2}], \qquad a_1 = 2(A^2 - B^2 + AB),$$

$$a_2 = \Delta(A+B), \quad a_3 = (B + 2A), \quad a_4 = 5B^2, \quad a_5 = \Delta B(2A + 6B),$$

$a_6 \equiv (\Delta A + \Delta B)^2$ and $\zeta(2r)$ is the zeta function of order $2r$. Thus the total carrier contribution to $\overline{\Delta} C_{44}$ and $\overline{\Delta} C_{456}$ in ultrathin films of p-type can, respectively, be expressed as

$$\overline{\Delta} \overline{C}_{44} = (-a_0^2/18\pi d_x)\,[C^{-1} \sum_{n_1=1}^{n_{1max}} (A_1'(E_F) + A_2'(E_F)) +$$

$$+ a_1^{-1} \sum_{n_2=1}^{n_{2max}} (A_3'(E_F) + A_4'(E_F)) + a_1^{-1} \sum_{n_3=1}^{n_{3max}} (A_5'(E_F) + A_6'(E_F))] \tag{6}$$

and

$$\overline{\Delta} C_{456} = (a_0^3/54 d_x)\,[C^{-1} \sum_{n_1=0}^{n_{1max}} (A_1''(E_F) + A_2''(E_F)) + a_1^{-1} \sum_{n_2=0}^{n_{2max}} (A_3''(E_F) +$$

$$+ A_4''(E_F)) + a_1^{-1} \sum_{n_3=0}^{n_{3max}} (A_5''(E_F) + A_6''(E_F))] \tag{7}$$

where single and double dashes denote the single and double differentiation with respect to E_F.

The thermoelectric power in the classically large magnetic field (G) which does not change the density-of-states function can be expressed, for the present case as[6],

$$G = S_0/ep_0 \tag{8}$$

where S_0 is the entropy. Thus combining Eqs. (1), (2) and (8) we get

$$\overline{\Delta} C_{44} = -a_0^2 p_0 Ge/3\pi^2 k_B^2 T \tag{9}$$

$$\overline{\Delta} C_{456} = (a_0^{33} ep_0 G^2/\pi^4 k_B^3 T)\left[3^{-1} + (p_0/3G)\left(\frac{dG}{dp_0}\right)\right]. \tag{10}$$

Thus we can express $\overline{\Delta} C_{44}$ and $\overline{\Delta} C_{456}$ by knowing G and its derivative.

Using the appropriate equations together with the parameters[7] $A = (-4.28\,\hbar^2/2m_0)$, $B = 2^{-1}(0.75\,\hbar^2/m_0)$, $\Delta = 0.033$ V, $T = 4.2$ K we have plotted the normalized $\overline{\Delta} C_{44}$ and $\overline{\Delta} C_{456}$ in ultrathin films of p-Si as functions of p_0 and d_x as shown in Figs. 1 and 2, respectively. It appears from both the figures. that $\overline{\Delta} C_{44}$ and $\overline{\Delta} C_{k56}$ increase with increasing p_0 and decrease with increasing d_x, respectively.

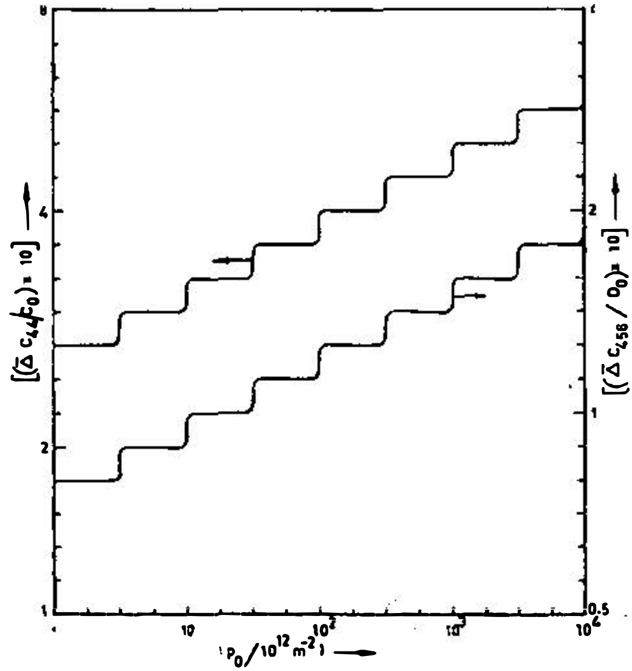

Fig. 1. Plots of normalized $\bar{\Delta} C_{44}$ and $\bar{\Delta} C_{456}$ versus p_0 in ultrathin films of p-Si (d_x = 40 nm).

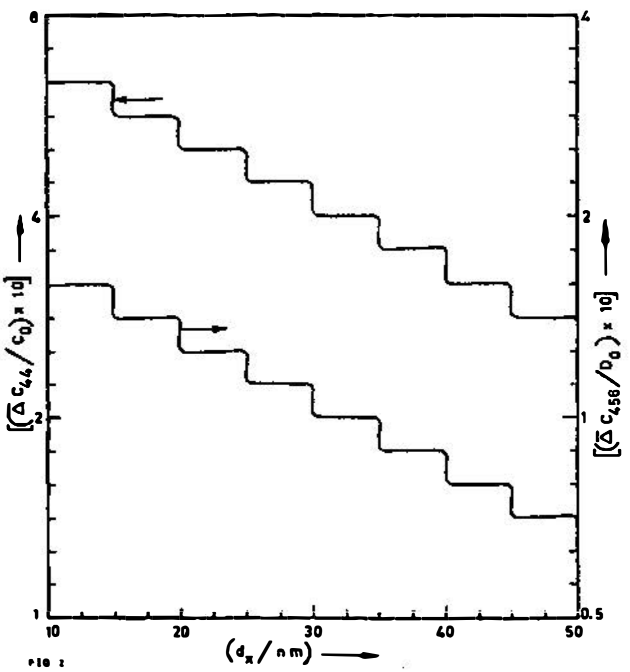

Fig. 2. Plots of normalized $\bar{\Delta} C_{44}$ and $\bar{\Delta} C_{456}$ versus d_x in ultrathin films of p-Si ($p_0 = 10^{14}\,m^{-2}$). The dotted plots exhibit the parabolic films of ultrathin films.

With varying p_0 and d_x a change is reflected in $\bar{\Delta}C_{44}$ and $\bar{\Delta}C_{456}$ through the redistribution of the electrons in the size quantized levels. The humps occur when the quantum numbers change from one set of fixed values to another allowed one. Since the experimental curve of G versus n_0 in the present case is not known to the best of our knowledge, we can not compare our theoretical formulation with the proposed experimental method of determining the electronic contribution to the elastic constants in ultrathin films. It may finally be suggested that experiments on the sound velocity involving the shear mode as a function of p_0 may exhibit the carrier contribution to the elastic constants of ultrathin films of p-Si which is our another experimental suggestion for determining $\bar{\Delta}C_{44}$ and $\bar{\Delta}C_{456}$, respectively.

References

1) M. Tsuchiya, J. M. Gaines, R. H. Yan, R. J. Simes, P. O. Holtz, L. A. Coldren and P. M. Petroff, Phys. Rev. Letts. **62** (1989) 466;

2) M. T. Linch, Festkörperprobleme **23** (1983) 227;

3) B. Mitra and K. P. Ghatak, Phys. Letts. **141A** (1989) 81 and the references cited therein;

4) K. P. Ghatak, S. Bhattacharyya and B. Mitra, Fizika **22** (1990) 489 and the references cited therein;

5) N. S. Averkiev, Yu. V. Ibisavskiy and V. M. Sternin, Solid State Commun. **52** (1984) 17;

6) T. M. Tsidilkovski, *Band Structure of Semiconductors* (Pergamon Press, London 1982);

7) N. Newberger, *Electronic Materials*, Plenum Data Corporation, New York, 1971.

O ELEKTRONSKOM DOPRINOSU ELASTIČNIM KONSTANTAMA VRLO TANKJH SLOJEVA p-TIPA Si

KAMAKHYA PRASAD GHATAK

Dept. of Electronics and Teleccm. Engineering, University of Jadavpur, Calcutta — 700 032, India

i

BADAL DE

Dept. of Electrical Engineering, John Brcwn E and Circ., 333 Udlow Street, P. O. Box 1422, Connecticut — 0690, USA

UDK 538.975

Originalni znanstveni rad

Razmatran je utjecaj teških, lakih i ultralakih šupljina na elastične konstante vrlo tankih slojeva p-tipa silicija. Sugerirana je eksperimentalna metoda za određivanje elastičnih konstanti u degeneriranim materijalima s proizvoljnim zakonom disperzije. Konstante elastičnosti rastu oscilatorno s porastom koncentracije šupljina, a opadaju porastom debljine filma.