Pressure and temperature derivatives of the elastic moduli of some polycrystalline semiconducting compounds using singlecrystal thirdorder elastic constant data and the elasticconstant pressure derivatives

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Pressure and temperature derivatives of the elastic moduli of some polycrystalline semiconducting compounds using single-crystal third-order elastic constant data and the elastic-constant pressure derivatives

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The pressure and the temperature derivatives of the bulk, shear, and Young's moduli and of the Poisson's ratio of some 3-5 and 2-6 polycrystalline semiconducting compounds have been calculated from Hill's approximation. The third-order elastic constants and the pressure derivatives of the second-order elastic constants of the corresponding single-crystal compounds have been employed in these calculations. Since the single-crystal input data are experimental, we would expect the present polycrystalline calculations to correspond to experimental measurements.

The calculation of the elastic properties of polycrystals from a knowledge of the elastic moduli and their pressure derivatives of the corresponding single crystals is quite an involved problem and has engaged the attention of many authors in the past. Voigt's[1] procedure of averaging the elastic stiffness tensor C_{ijkl} is based on the assumption of uniform state of strain in the crystal, while the Reuss procedure[2] of averaging the compliance tensor S_{ijkl} is consistent with the assumption of uniform state of stress in the crystal. Both these methods are used to obtain the polycrystal elastic moduli B, G, and E, and the Poisson's ratio σ. If the polycrystal is considered as an aggregate of randomly oriented crystals, then it can be replaced by an equivalent isotropic and homogeneous elastic body, and the Voigt and Reuss limits constitute the upper and lower bounds, respectively. However, except for the case when the anisotropy of the crystal is small, these bounds are not close enough to provide a good estimate for the effective elastic moduli, and in fact, the Voigt and Reuss averages represent the first-order bounds. Based on the energy argument, Hill[3] suggested that the arithmetic mean of the Voigt and the Reuss limits be used to express the most probable value for the polycrystalline solid. Hashin and Shtrikman,[4] using a variational approach, obtained the second-order bounds for cubic symmetry, while Kroner and Koch[5] obtained third-order bounds. Gairola and Kroner[6] proposed a formulation for calculating all the bounds and the self-consistent value of the shear modulus of a cubic polycrystal. Peresada[7] proposed a new method to estimate the elastic moduli of a polycrystal from single-crystal data of any symmetry, which leads to results in good agreement with those obtained by Hill's[3] approximation.

The 3-5 compounds GaAs, GaSb, and InSb, and the 2-6 compounds ZnSe and ZnTe are elastically isotropic to a large extent, as indicated by the elastic anisotropic index $(2C_{44}/C_{11}-C_{12})$. As such, the Hill's[3] procedure is well suited to obtain the elastic moduli of the polycrystalline compounds of these materials. The pressure derivative of the shear modulus of a polycrystal is an experimentally measured quantity, and hence, it is of interest to obtain the same derivative, theoretically. In this paper, the pressure derivatives of the elastic moduli and of the Poisson's ratio of the polycrystalline solids of these semiconducting compounds are calculated using either the third-order elastic constants (TOEC) or the pressure derivatives of the second-order elastic constants (SOEC) of the corresponding single crystal. The temperature variation of the elastic moduli of the polycrystalline compounds is also presented.

In the Voigt's scheme, the bulk (B_V) and the shear (G_V) moduli of cubic materials are given by

$$3B_V = C_{11} + 2C_{12} \tag{1}$$

and

$$5G_V = (C_{11} - C_{12} + 3C_{44}) . \tag{2}$$

In the Reuss scheme, these are given by

$$B_R^{-1} = 3(S_{11} + 2S_{12}) \tag{3}$$

and

$$5G_R^{-1} = 4(S_{11} - S_{12}) + 3S_{44} . \tag{4}$$

The compliance coefficients S_{ij} are related to the stiffness coefficients C_{ij} in the cubic case, as

$$S_{11} = (C_{11} + C_{12})/(C_{11} - C_{12})(C_{11} + 2C_{12}) , \tag{5}$$

$$S_{12} = -C_{12}/(C_{11} - C_{12})(C_{11} + 2C_{12}) , \tag{6}$$

and

$$S_{44} = 1/C_{44} . \tag{7}$$

Poisson's ratio σ and Young's modulus E, with the values of B and G determined by Voigt's or Reuss' averaging procedures, can be calculated from

$$2\sigma = 3B - 2G/3B + G \tag{8}$$

and

$$9E^{-1} = 3G^{-1} + B^{-1} . \tag{9}$$

In the Hill approximation, one writes

$$2M_H = M_V + M_R , \tag{10}$$

where M_H, M_V, and M_R represent the Hill, Voigt, and Reuss averages, respectively, of any elastic quantity. The pressure derivatives B'_V, G'_V, B'_R, G'_R, σ', and E' are obtained using formulas (1)–(9).

$$3B'_V = C'_{11} + 2C'_{12} , \tag{11}$$

$$5G'_V = C'_{11} - C'_{12} + 3C'_{44} , \tag{12}$$

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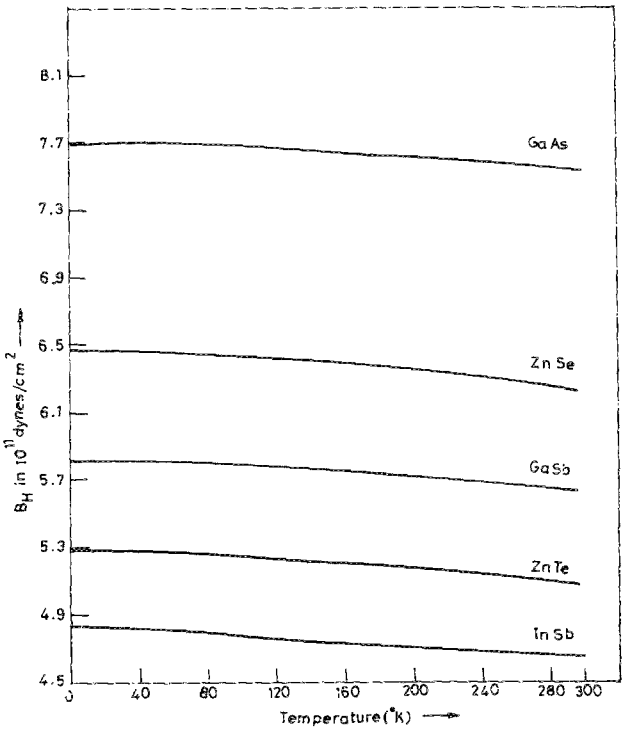

FIG. 1. Variation of the polycrystal bulk modulus with temperature.

$$B'_R = -3B_R^2(S'_{11} + 2S'_{12}), \tag{13}$$

$$5G'_R = -G_R^2[4(S'_{11} - S'_{12}) + 3S'_{44}], \tag{14}$$

$$\sigma' = [1/2(3B+G)^2][(3B+G)(3B'-2G') - (3B-2G)(3B'+G')], \tag{15}$$

$$E' = (E^2/9)[(3G'/G^2) + (B'/B^2)], \tag{16}$$

where C'_{ij} means dC_{ij}/dp and a similar connotation for the other dashed quantities.

The pressure derivatives of the bulk, shear, and Young's moduli and of the Poisson's ratio of five semiconducting

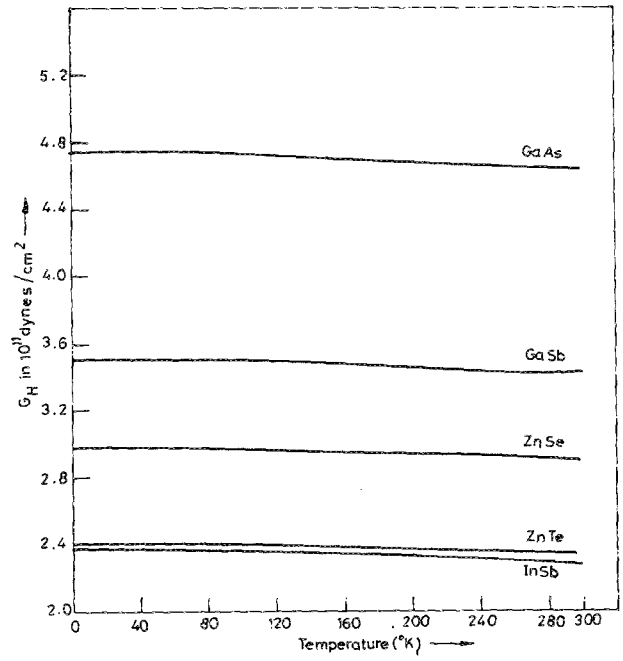

FIG. 2. Variation of the polycrystal shear modulus with temperature.

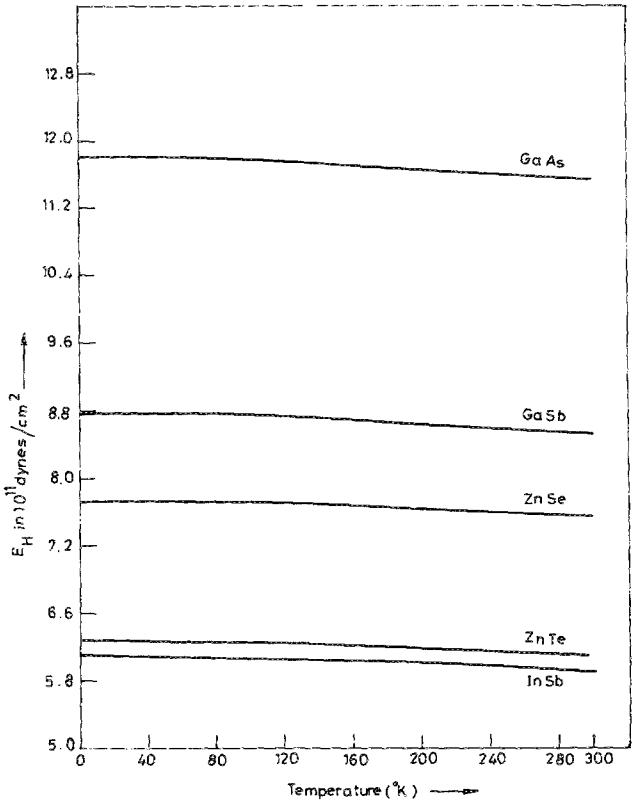

FIG. 3. Variation of the polycrystal Young's modulus with temperature.

polycrystalline compounds have been calculated using either the third-order elastic constants (TOEC) or the pressure derivatives of the second-order elastic constants (SOEC) of the corresponding single crystals. The experimental TOEC of the single-crystal GaAs (Ref. 8), GaSb (Ref. 9), and InSb (Ref. 10), and the experimental pressure derivatives of the SOEC of ZnSe (Ref. 11) and ZnTe (Ref. 11) are available in the literature. The values of B, G, and E of the polycrystal at various temperatures are calculated from a knowledge of the temperature variation of the SOEC of the corresponding single crystal. The temperature variation of the SOEC of GaAs (Ref. 12), GaSb (Ref. 13), InSb (Ref. 14), and ZnTe (Ref. 15) and ZnSe (Ref. 15) is used to obtain the elastic moduli of the corresponding polycrystals at various temperatures. The variations of B, G, and E of the polycrystalline compounds with temperature are shown in Figs. 1, 2, and 3, respectively. The temperature derivatives of B, G, and E at room temperature are calculated from the graphs and are presented in Table I. Following Guinan and

TABLE I. Temperature derivatives of B, G, and E at room temperature. The units of the temperature derivative of the elastic modulus are 10^{11} dyn/cm^2 K and the temperature derivatives are denoted by $\overline{B}_H$, $\overline{G}_H$, and $\overline{E}_H$ (e.g., $\overline{B}_H = dB_H/dT$).

Compound	$10^3 \times \overline{B}_H$	$10^3 \times \overline{G}_H$	$10^3 \times \overline{E}_H$
GaAs	0.87	0.43	0.87
GaSb	0.50	0.30	0.50
InSb	0.45	0.35	1.25
ZnTe	1.14	0.29	0.86
ZnSe	1.43	0.29	1.14

TABLE II. The values of B'_H, G'_H, E'_H, and σ'_H in Voigt, Reuss, and Hill's approximations. The first row of each compound gives the Voigt's bounds, the Reuss bounds are given in the second row, and the values in the Hill's approximation are given in the third row.

No.	Compound		B'_H	G'_H	E'_H	$\sigma'_H \times 10^{11}$
1.	GaAs	(i)	4.52	0.71	2.71	0.099
		(ii)	4.52	0.46	2.06	0.102
		(iii)	4.52	0.585	2.39	0.101
2.	GaSb	(i)	4.76	0.66	2.64	0.142
		(ii)	4.76	0.44	2.07	0.145
		(iii)	4.76	0.55	2.36	0.144
3.	InSb	(i)	3.97	0.18	1.17	0.147
		(ii)	3.97	−0.003	0.64	0.149
		(iii)	3.97	0.089	0.91	0.148
4.	ZnTe	(i)	5.02	0.21	1.35	0.163
		(ii)	5.02	0.003	0.73	0.163
		(iii)	5.02	0.107	1.04	0.163
5.	ZnSe	(i)	4.77	0.16	1.24	0.132
		(ii)	4.75	−0.11	0.41	0.132
		(iii)	4.76	0.025	0.825	0.132

Steinberg,[16] we have used the direct pressure derivative approach in these calculations. The values of the pressure derivatives of the elastic moduli of the polycrystals are presented in Table II, and this data would be useful from a technical viewpoint. From Table II we find that the pressure derivatives of the bulk modulus and the Poisson's ratio have nearly the same limits, while those of shear and Young's moduli have widely differing limits in both the procedures. InSb and ZnSe, in fact, have negative pressure derivatives of the shear modulus in the Reuss procedure. However, in the Hill approximation, the pressure derivatives of the elastic moduli of all five of these compounds are positive.

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[1]W. Voigt, Ann. Phys. **38**, 573 (1889).
[2]A. Reuss, Z. Angew. Math. Mech. **9**, 49 (1929).
[3]R. Hill, Proc. Phys. Soc. (London) A **65**, 349 (1952).
[4]Z. Hashin and S. Shtrikman, J. Mech. Phys. Solids **10**, 335 (1962).
[5]E. Kroner and H. Koch, Solid Mech. Arch. **1**, 183 (1976).
[6]B. K. D. Gairola and E. Kroner, Int. J. Eng. Sci. **19**, 865 (1981).
[7]G. I. Peresada, Phys. Status Solidi A **4**, K23 (1971).
[8]H. J. McSkimin and P. Andreatch, Jr., J. Appl. Phys. **38**, 2610 (1967).
[9]V. Sundara Raja and P. J. Reddy, Phys. Lett. A **56**, 215 (1976).
[10]J. R. Drabble and A. J. Brammer, Proc. Phys. Soc. **91**, 959 (1967).
[11]B. H. Lee, J. Appl. Phys. **41**, 2988 (1970).
[12]R. I. Cottam and G. A. Saunders, J. Phys. C **6**, 2105 (1973).
[13]J. T. Lin and C. Wong, J. Phys. Chem. Solids **33**, 241 (1972).
[14]L. J. Slutsky and C. W. Garland, Phys. Rev. **113**, 167 (1959).
[15]B. H. Lee, J. Appl. Phys. **41**, 2984 (1970).
[16]M. W. Guinan and D. J. Steinberg, J. Phys. Chem. Solids **35**, 1501 (1974).

A local measurement of Ba^+ density temporal evolution

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The local temporal evolution of the Ba^+ number density in a resonant laser-driven barium plasma has been measured for the first time by using near-resonance Rayleigh scattering. This local temporal evolution is quite different from other measurements, where spatially integrated absorption methods were employed.

In recent years laser-driven resonant ionization has been demonstrated to be an efficient technique to generate plasmas.[1–7] The mechanism for this ionization, although extremely complicated, can be characterized by a few processes,[8] among which superelastic collisions[9] are believed to be dominant. Due to the nonequilibrium characteristics of the plasma, a measurement of the spatially resolved temporal evolution of the ionization is necessary; however, so far only line-averaged measurements have been made.[4,5]

We have measured the Ba^+ number density and its temporal evolution by near-resonant Rayleigh scattering (NRRS). The advantage of this method over other techniques lies in its spatial resolution. These measurements can provide useful information about the ionization processes in this kind of laser-vapor interaction.

The experimental setup and the absolute calibration of the NRRS signals are discussed in this communication. Experimental results, analysis, and comparisons with other measurements are also given.

The plasma source is a barium heat-pipe oven, as shown in Fig. 1. The oven is filled with 25 Torr of argon to protect the windows from the hot barium. Barium ions are generated by illuminating the Ba vapor with a flashlamp-pumped dye laser (referred to as a pump laser) tuned to Ba I resonance transition $6s^2\ ^1S_0 - 6s6p\ ^1P_1$, $\lambda = 553.55$ nm. This laser produces a 1-μs-long pulse of 200-mJ energy, with a 0.3-nm bandwidth and a 2.5-cm beam diam. The Ba^+ number density is measured by another tunable dye laser (referred to as a probe laser) pumped by a Nd:YAG laser. The probe laser is tuned near the Ba^+ resonance transition $6s^2S_{1/2} - 6p^2P_{1/2}$, $\lambda = 493.41$ nm, with an energy of 1 mJ and a bandwidth of 2.5×10^{-3} nm. A dichroic mirror is used to superimpose the two laser beams. The timing between two

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