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Elastic Moduli of Gallium Antimonide under Pressure and the Evaluation of Compression to 80 kbar

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Ultrasonic wave velocities in GaSb have been measured at 25°C as a function of hydrostatic pressure to 2 kbar. The adiabatic "zero-field" stiffness moduli calculated from these velocities (for 1 atm) are as follows: $c_{11}=8.839\pm0.008$, $c_{12}=4.033\pm0.010$, $c_{44}=4.316\pm0.004$, and B_s (bulk modulus) $=5.635\pm.012$. All moduli are in units of 10^{11} dyn/cm^2 and are based on a density of 5.6137 g/cm^3 taken as exact with respect to estimates of errors. Hydrostatic pressure derivatives for c_{11}, c_{12}, c_{44}, and B_s are, respectively, 4.96 ± 0.10, 4.64 ± 0.15, 1.01 ± 0.02, and 4.75 ± 0.15. The static compression of GaSb to 80 kbar has been evaluated using the isothermal bulk modulus (B_T) of 5.614×10^{11} dyn/cm^2 and $(\partial B_T/\partial P)$ of 4.78.

I. INTRODUCTION

In a recent publication[1] we reported the pressure variations of the second-order elastic moduli of GaAs and evaluated the compression to 250 kbar using a method suggested by Anderson.[2] We were motivated to undertake a similar study on GaSb because of the continuing interest in elastic properties of group III–V semiconductor compounds under pressure.

Measurements for the second-order moduli at 1 atm and ~300°K have been reported by McSkimin *et al.*[3] and by Bolef and Menes[4] (c_{11} and c_{44} only). To our knowledge, however, no data on the pressure variations of the elastic moduli of GaSb have been reported in the literature.

II. EXPERIMENTAL METHODS AND RESULTS

Ultrasonic wave velocities from which the moduli could be computed were measured at 40 MHz by means of a pulse superposition technique which has been described previously.[5]

The GaSb specimen was n-type Te doped ($n=3\times10^{18}$) and had an electrical resistivity of 0.0065 Ω·cm at room temperature, adequately low to insure zero-field propagation conditions for this piezoelectric material. Faces parallel to (110) and (100) planes of the crystal were ground from a sample whose growth direction was along the [110] direction. All surfaces were polished, and flat to within ¼ wavelength of sodium light. Corresponding faces were parallel to within 10 sec of arc, with crystallographic orientations held within 20 min for the [001] and [110] directions. Dimensions were 0.81064 cm in [001] direction, and 0.90734 cm in [110].

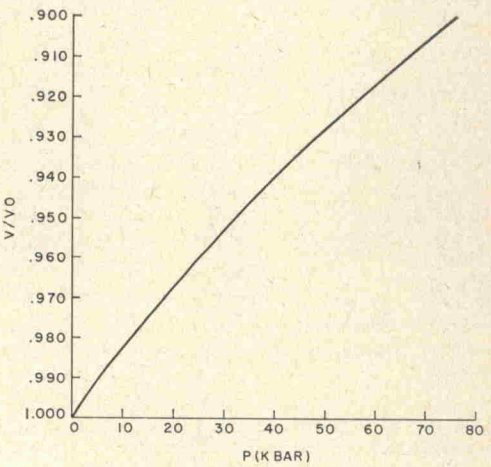


FIG. 1. Pressure–volume relationship for GaSb at 25°C.

Table I lists measured values of frequency ratios f_R/f_{R_0} (reciprocal delay times), where f_R is the value at 30 000 psi and f_{R_0} is the value at 0 excess pressure. The velocities for these two pressures are also shown. The second-order stiffness moduli and their pressure derivatives are shown in Table II. A density of 5.6137

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TABLE I. Measured f_R/f_{R_0} ratios at 30 000 psi and wave velocities for GaSb at 25°C.

Designation	Mode	Propagation direction	Displacement direction	f_R/f_{R0} ($p=30\,000$ psi)	Velocity[a] $p=0$ (units of 10^5 cm/sec)	Velocity $p=30\,000$ psi (units of 10^5 cm/sec)
V_1	Long.	001	001	1.005164	3.96807	3.98368
V_2	Shear	001	110	1.001796	2.77291	2.77449
V_3	Long.	110	110	1.005028	4.37617	4.39279
V_4	Shear	110	001	1.001794	2.77244	2.77401
V_5	Shear	110	$1\bar{1}0$	1.000059	2.06901	2.06660

[a] Estimated uncertainty = 0.05%.

g/cm³ at 25°C was used, as determined from lattice constants by Straumanis and Kim.[6]

In Table III the second-order moduli obtained in the present study are compared with previous results.

III. COMPRESSION TO 80 kbar

Using the method suggested by Anderson,[2] we have evaluated the static compression of GaSb to 80 kbar. The isothermal bulk modulus (B_T) and its pressure derivative ($\partial B_T/\partial P$) needed for the computation were calculated from the measured adiabatic values, using the relations given by Anderson. In this connection, one needs to know the thermal Grüneisen constant γ, the volume thermal expansion coefficient α_v, its variation with temperature $(\partial\alpha_v/\partial T)_p$, and $(\partial B_T/\partial T)_p$, the temperature derivative of the bulk modulus. We obtained α_v from the measured linear expansion coefficient of $\alpha=6.3\times10^{-6}$/°C,[7] γ of 0.68[8] and used an estimated value of 1×10^{-8} for $(\partial\alpha_v/\partial T)_p$.[7] From the experimentally determined adiabatic bulk modulus $B_s=563.49$ kbar and its pressure derivative $B_s'=4.75$ and $(\partial B_s/\partial T)_p=0.07$ kbar/°C, the isothermal bulk modulus of 561.44 kbar, and $B_T'=4.78$ were obtained and used in the computation. Figure 1 shows the pressure–volume relationship computed using the Birch equation of state. The numerical data are given in Table IV. The pressure–volume relationship obtained using the Murnagham equation of state shows no observable deviation from the data of Fig. 1. Since GaSb is known to undergo a pressure induced phase transformation to white-tin type structure[9,10] at about 80 kbar, evaluation of compression was limited to this pressure.

TABLE II. Elastic moduli at 25°C and their pressure derivatives.

Formula	Value at $p=0$[a]	Value at $p=30\,000$ psi[a]	Pressure derivative
$c_{11}=\rho V_1^2$	8.8391	8.9416	4.96
$c_{11}=\rho(V_5^2+V_3^2-V_4^2)$	8.8389	8.9431	5.04
$c_{12}=\rho(V_1^2-2V_5^2)$	4.0329	4.1289	4.64
$c_{12}=\rho(V_3^2-V_5^2-V_4^2)$	4.0327	4.1304	4.72
$c_{44}=\rho V_2^2$	4.3164	4.3372	1.01
$c_{44}=\rho V_4^2$	4.3149	4.3357	1.01
$B_s=\frac{1}{3}(c_{11}+2c_{12})$	5.6349	5.7331	4.75

[a] Units of 10^{11} dyn/cm², pressure is excess over 1 atm, density used is 5.6137 g/cm³.

TABLE III. Comparison of second-order moduli of GaSb.

Modulus[a]	Bolef and Menes[b] (1960)	McSkimin *et al.*[c] (1956)	McSkimin *et al.*[d] (present study)
c_{11}	8.840	8.841	8.839
c_{12}	...	4.033	4.033
c_{44}	4.319	4.321	4.316

[a] Values are shown in units of 10^{11} dyn/cm².
[b] 30 MHz values, $T=27$°C, $\rho=5.619$.
[c] Values recalculated using density = 5.6317 g/cm³, $T=25$°C.
[d] Based on density of 5.6317 g/cm³, $T=25$°C.

TABLE IV. Compression data for GaSb ($T=25$°C).

P(kbar)	V/V_0	P(kbar)	V/V_0
2.84	0.995	44.32	0.935
5.78	0.990	46.80	0.932
8.8	0.985	48.47	0.930
11.9	0.980	51.02	0.927
15.1	0.975	52.75	0.925
18.4	0.970	55.38	0.922
21.78	0.965	57.16	0.920
23.86	0.962	59.86	0.917
25.27	0.960	61.70	0.915
27.41	0.957	64.48	0.912
28.86	0.955	66.37	0.910
31.06	0.952	69.24	0.907
32.55	0.950	71.18	0.905
34.83	0.947	74.14	0.902
36.36	0.945	76.14	0.900
38.70	0.942	79.19	0.897
40.28	0.940	80.22	0.896
42.69	0.937		

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