

ELASTICITY MODULI OF $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ SOLID SOLUTIONS

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Results of investigations into the temperature dependences (4.2–300 K) of the low-frequency ultrasound velocity in $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ single crystals are presented. The elastic moduli and the Debye temperatures are calculated for different solid solution compositions. Based on the data obtained, possible stresses are estimated on the heteroboundary of the materials with a number of substrates.

Keywords: solid solutions, elasticity moduli, temperature dependences.

In 2009, 50 years passed since synthesis of the $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ solid solution. During this time, several ten thousand works devoted to the study of methods of synthesis of the material and its properties and to the development of different instruments on its basis have been published, numerous conferences and seminars have been held, and recognized monographs have been written. Nevertheless, a number of gaps still exist even in the materials science devoted to this solid solution. Among them are the elasticity moduli of this solid solution. Except [1, 2] devoted to two $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ compositions, we do not aware of any other direct measurements of its elastic properties. This situation is also typical for other solid solutions of A^2B^6 compounds. In our opinion, this is explained by two circumstances. First, the complexity of the corresponding investigations should be mentioned. To study the elastic properties of semiconductor materials by the conventional acoustic methods, sufficiently large oriented single crystals with homogeneous composition are required. The accuracy of measurements of the ultrasound velocity on a level of 10^{-4} – 10^{-5} is conventionally reached for samples whose thickness and transverse dimensions are of the order of a centimeter. It is difficult to grow such crystals of solid solutions, and inhomogeneity of their composition is inevitable irrespective of the growth method. Second, when the necessity arises to use elasticity moduli of solid solutions, estimates representing linear extrapolation of the corresponding moduli for binary compounds forming the solid solution are often used. This can give significant errors.

In the present work, results of investigations into the velocity of ultrasound wave propagation are given that allow the elasticity moduli to be calculated for a number of $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ solid-solution compositions. The examined single crystals were grown by the method of vertical directed crystallization from the solid phase, which allowed samples with homogeneous composition to be synthesized with controllable levels of residual native defects. To decrease the level of defects, the crystals were doped by indium to a level of 10^{14} cm^{-3} that had no effect on the electrophysical parameters of the material. Crystals used for measurements were shaped as discs or plane-parallel plates with sizes from 1 to 1.5 cm and thickness of about 0.1 cm. The normals to the plane sample surfaces and hence the directions of ultrasound propagation coincided with one of the [100], [110], and [111] crystallographic directions. Misorientation with respect to the indicated directions did not exceed 2° . To obtain plane-parallel surfaces, the central regions of preliminary oriented grinded and etched large (about 3 cm in diameter) plates were used.

Plates with the above-indicated dimensions are optimal for excitation in them of ultrasound waves by the method of direct conversion of electromagnetic and acoustic waves in a constant magnetic field [3]. To increase the efficiency of electromagnetic-acoustic conversion in the semiconductor material, aluminum layers with thickness of

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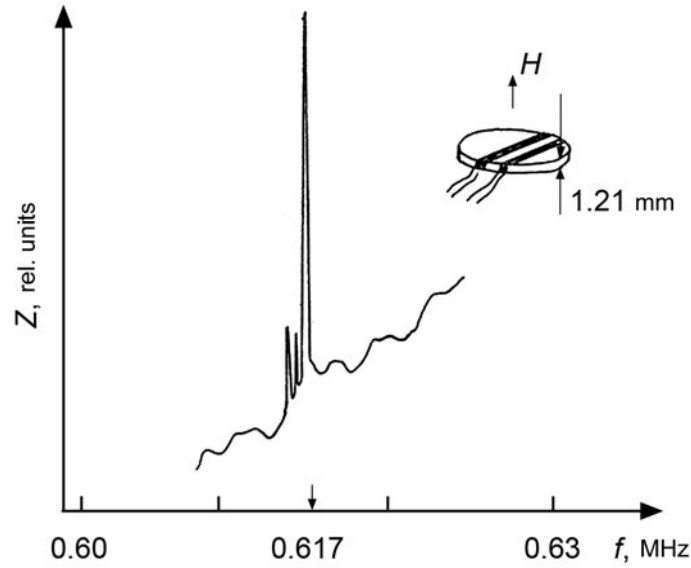


Fig. 1. Resonant curve for the crystal with $\text{Cd}_{0.3}\text{Hg}_{0.7}\text{Te}$ composition at a temperature of 4.2 K. The geometry of coils used for excitation and registration of ultrasonic oscillations is shown in the insert.

about $1\text{ }\mu\text{m}$ were deposited in vacuum on the preliminary prepared crystal surface. Coils were placed above the aluminum layer and sample (see the insert in Fig. 1), one of which was operated from a high-frequency voltage. Alternating current j was induced in the aluminum layer. The Lorentz interaction with the electron subsystem of the examined sample was observed in the external constant magnetic field H . It can be described by the equation for the Ampere force:

$$F_L = [j, H] / c,$$

where c is the velocity of light. In this case, the Lorentz force acts on free carriers. If the vector H is perpendicular to the plate, the Lorentz force lies in the plate plane. In this case, transverse sound waves propagating through the semiconductor crystal volume are excited in the Al film whose thickness is close to that of the skin layer. When the orientation of the magnetic field H is parallel to the sample plane, longitudinal sound waves are excited in the sample. The direction of the ultrasound velocity vector in this case coincides with the [011] or [111] symmetry axis of the semiconductor lattice. The ultrasound wave was detected with the use of the electromagnetic-acoustic conversion effect in the second coil having a rectangular cross section placed above the sample surface. The sample and two coils – primary and secondary – were put in a cryostat with adjustable temperature chamber filled with liquid helium. The external magnetic field $H \approx 8\text{ T}$ was created by a superconducting solenoid. Measurements were performed at temperatures in the range 4–250 K.

Under conditions of our experiment, a standing acoustic wave was formed in the plane-parallel sample. Its wavelength λ is related to the frequency f of the alternating current in the skin layer by the expression $\lambda = 2DS / f$, where S is the velocity of sound and D is the transverse plate size. Resonant changes in the total surface plate impedance Z were observed at the frequencies corresponding to excitation of standing ultrasound waves. These changes were registered by the standard radio engineering methods. The frequencies of the Fabry–Perot acoustic resonances in the plate are determined by the formula

$$f_{l,t} = nS_{l,t} / 2D, \quad n = 1, 3, 5, 7, \dots,$$

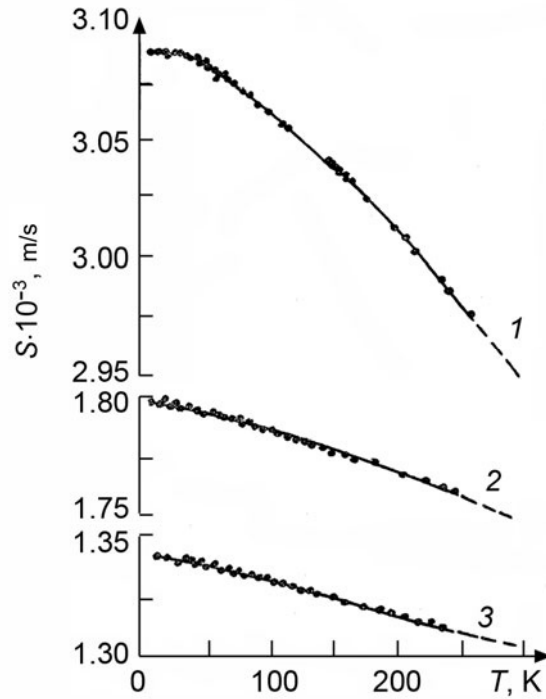


Fig. 2. Temperature dependences of the velocities of longitudinal ultrasound (curve 1) and transverse ultrasound with two polarization states (curves 2 and 3) propagating in the $\text{Cd}_{0.21}\text{Hg}_{0.79}\text{Te}$ single crystal.

where the subscripts l and t designate the longitudinal and transverse polarization states of ultrasound waves, respectively. The ultrasound wave velocities were determined by this method with accuracy of 10^{-3} . Measurements were performed in the range $2.5 \cdot 10^6 - 1.5 \cdot 10^7 \text{ s}^{-1}$ at frequencies of the first ($n = 1$) Fabry–Perot longitudinal and transverse ultrasound wave resonances. In some cases, test measurements at frequencies of the subsequent ($n = 3$ and 5) resonances were performed. The typical resonant curve is shown in Fig. 1.

In this work, ultrasound investigations of seven solid-solution compositions were performed, and only for three of them, the surface orientation corresponded to the $[110]$ direction for which the velocities of longitudinal and two transverse ultrasound waves were measured. This was sufficient for calculation of all moduli of rigidity C_{11} , C_{12} , and C_{44} for the examined material. The temperature dependences of the longitudinal and transverse elastic wave velocities for the sample with $x = 0.21$ is shown in Fig. 2. For the ultrasound waves propagating in these directions, the measured sound velocities were related to the sought-after elastic moduli by the following expressions:

$$\begin{aligned} \rho S_l^2 &= (C_{11} + C_{12} + 2C_{44}) / 2, \\ \rho S_{tl}^2 &= (C_{11} - C_{12}) / 2, \\ \rho S_{t2}^2 &= C_{44}. \end{aligned} \quad (1)$$

Here ρ is the material density. Tables 1–3 tabulate the moduli of rigidity C_{ij} for the examined materials together with some other characteristics calculated from them, including the anisotropy factor B , the Young modulus E , the Poisson coefficient ν , and the isothermal bulk modulus K :

$$B = 2C_{44} / (C_{11} - C_{12}),$$

TABLE 1. Cd_{0.11}Hg_{0.89}Te Elastic Parameters

T, K	$C_{11} \cdot 10^{10}, Pa$	$C_{12} \cdot 10^{10}, Pa$	$C_{44} \cdot 10^{10}, Pa$	$B \cdot 10^{10}, Pa$	$\nu \cdot 10^{10}, Pa$	$E \cdot 10^{10}, Pa$	$K \cdot 10^{10}, Pa$
4	64.5	42.3	25.9	2.33	0.396	31.1	49.7
20	64.5	42.2	25.9	2.32	0.396	31.1	49.6
78	63.9	41.6	25.6	2.29	0.394	31.2	49.0
100	63.5	41.3	25.5	2.29	0.394	31.0	48.7
150	62.6	40.6	25.2	2.30	0.394	30.6	47.9
200	61.5	39.8	25.0	2.31	0.394	30.1	47.0
250	60.3	39.0	24.6	2.31	0.393	29.6	46.1
300*	59.0	38.1	24.3	2.32	0.392	29.1	45.1

TABLE 2. Cd_{0.21}Hg_{0.79}Te Elastic Parameters

T, K	$C_{11} \cdot 10^{10}, Pa$	$C_{12} \cdot 10^{10}, Pa$	$C_{44} \cdot 10^{10}, Pa$	$B \cdot 10^{10}, Pa$	$\nu \cdot 10^{10}, Pa$	$E \cdot 10^{10}, Pa$	$K \cdot 10^{10}, Pa$
4	61.8	34.3	24.6	1.79	0.357	37.3	43.5
20	61.7	34.2	24.6	1.79	0.357	37.3	43.4
78	61.1	33.9	24.4	1.79	0.357	36.9	43.0
100	60.8	33.6	24.3	1.79	0.356	36.8	42.7
150	59.7	32.8	24.1	1.79	0.355	36.3	41.8
200	58.5	31.9	23.9	1.79	0.353	36.0	40.8
250	57.2	30.9	23.7	1.80	0.351	35.5	39.6
300*	56.0	30.0	23.4	1.80	0.349	35.0	38.7

TABLE 3. Cd_{0.3}Hg_{0.7}Te Elastic Parameters

T, K	$C_{11} \cdot 10^{10}, Pa$	$C_{12} \cdot 10^{10}, Pa$	$C_{44} \cdot 10^{10}, Pa$	$B \cdot 10^{10}, Pa$	$\nu \cdot 10^{10}, Pa$	$E \cdot 10^{10}, Pa$	$K \cdot 10^{10}, Pa$
4	67.9	40.2	25.3	1.83	0.372	38.0	49.4
20	67.8	40.2	25.3	1.83	0.372	37.9	49.4
78	67.0	39.8	25.1	1.83	0.372	37.3	48.9
100	66.5	39.4	25.0	1.84	0.372	37.2	48.4
150	65.4	38.6	24.7	1.84	0.371	36.7	47.5
200	64.1	37.8	24.4	1.85	0.371	36.1	46.6
250	63.1	37.0	24.2	1.86	0.370	35.7	45.6
300	61.9	36.2	24.0	1.86	0.369	35.2	44.8

*The data for $T = 300$ K were obtained by extrapolation of the temperature dependences.

$$\nu = C_{12} / (C_{11} + C_{12}) \quad (2)$$

$$E = (C_{11}^2 - C_{12}^2) / (C_{11} + 2C_{12}),$$

$$K = (C_{11} + C_{12}) / 3.$$

Values of all above-indicated parameters are presented for temperatures in the range 4–300 K; the last value was obtained by linear extrapolation from the range 150–250 K.

The results obtained do not allow us to construct a dependence of the elasticity moduli for the solid solution versus its composition; however, their comparison with the corresponding parameters of the initial binary HgTe and CdTe compounds [6] demonstrates that the linear interpolation between the initial values is a very rough approximation.

TABLE 4. Calculated Mismatch Stresses in $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ Based Heterostructures

x	Substrate	CdTe	GaAs	InP	Si
0.21	ϵ_{xx}	-0.002676	0.011536	0.009015	0.014932
	ϵ_{zz}	0.000214	-0.000923	-0.000721	-0.001194
	σ_{xx} , kg/mm^2	8.664269	38.213327	29.865854	49.460870
0.3	ϵ_{xx}	-0.002330	0.011491	0.009028	0.014879
	ϵ_{zz}	0.000419	-0.002068	-0.001625	-0.002678
	σ_{xx} , kg/mm^2	-8.450207	41.672257	32.739647	53.955977

Because direct measurements of the elastic parameters for the examined solid solution were lacking, we undertook measures on checking the accuracy and reliability of the results obtained. Additional measurements of the longitudinal and transverse ultrasound velocities were performed for samples of the same compositions with $x = 0.21$ and two different orientations: [110] for which all three elasticity moduli were calculated from Eq. (1) and [111]. For the latter orientation, the velocities S_l and S_t are related to the elasticity moduli by expressions

$$\begin{aligned}\rho S_l^2 &= (C_{11} + 2C_{12} + 4C_{44})/3, \\ \rho S_t^2 &= (C_{11} - C_{12} + C_{44})/3,\end{aligned}\tag{3}$$

that allow only two their linear combinations to be calculated. The moduli C_{11} , C_{12} , and C_{44} calculated from measurements for the [110] orientation were substituted into Eq. (3), and the sound velocities so obtained were then compared with their values measured directly for the sample with the [111] orientation. Their comparison demonstrated that the calculated and measured velocities coincided within the experimental accuracy (about 1%) for the entire range of temperatures. This testifies to the reliability of the results obtained that can be compared only with the data of direct measurements of the $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ bulk modulus. The isothermal bulk moduli calculated from Eq. (2) for the composition with $x = 0.2$ were $K = (38.7 \pm 0.4) \cdot 10^{10} \text{ dyn/cm}^2$ for $T = 300 \text{ K}$. This is in fairly good agreement with the experimental data on hydrostatic compression with $K = (41 \pm 2) \cdot 10^{10} \text{ dyn/cm}^2$ [5]. The anisotropy factor $B = 2C_{44}/(C_{11} - C_{12})$ calculated from our measurements for $\text{Cd}_{0.21}\text{Hg}_{0.79}\text{Te}$ remained virtually unchanged for temperatures in the range 4–300 K and was much smaller (namely, $B = 1.79$) than for CdTe ($B = 2.43$) and HgTe ($B = 2.47$) [6]. This testifies to the reduced anisotropy of the elastic properties for the solid solution in comparison with the binary compounds and is most likely due to misorientation of the solid solution lattice.

We note also that the Debye temperatures calculated from our ultrasonic measurements of the elasticity moduli for $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ solid solutions are in reasonable agreement with the temperature obtained in [7] from the data of calorimetric measurements of the specific heat.

Thus, the elastic moduli for the $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ solid solution are in good agreement with other properties of the material crystal lattice. The results presented in this work allow deformations and stresses caused by them on the heteroboundaries of the epitaxial $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ layer with the single-crystal substrate to be estimated. Such estimates were obtained for compositions with $x = 0.21$ and 0.3 and a number of substrate materials under assumptions of rigid bonding and absence of intermediate layers. Results of calculations of the mismatch stresses (they were approximately 10 times greater than the thermoelastic stresses for the examined combinations of the materials in contact) are tabulated in Table 4.

It appears that the calculated deformations exceed by an order of magnitude the deformation actually observed in the examined structure: $\epsilon_{\text{theor}} = -0.002$ and $\epsilon_{\text{exp}} = -0.0006$, respectively. The last result was obtained by precision x-ray structural investigations on the boundary between the $\text{Cd}_{0.2}\text{Hg}_{0.8}\text{Te}$ epitaxial layer with thickness of $\sim 1 \mu\text{m}$ deposited on the CdTe oriented single-crystal substrate in low-temperature high-frequency mercury plasma [8].

The calculations described above were performed under assumption of rigid bonding of the substrate with the layer. This assumption is seldom realized in practice due to the graded-gap layer with intermediate structure formed

between the substrate and the film in the process of growth due to mutual diffusion of atoms of the incremental material and the substrate. The presence of transitive layers leads to significant stress relaxation on the heteroboundary, thereby reducing the stress several times.

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