ELASTIC CONSTANTS OF β-HgS*

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The elastic constants of single crystals of β-HgS highly doped with iron were directly determined at room temperature from the measurements of ultrasonic wave velocities by the pulse-echo technique. The values of $c_{11} = 6.750$, $c_{12} = 5.186$, and $c_{44} = 2.42$ (given at 10^{10} N m^{-2} units) were obtained and compared with the experimental data taken for other mercury chalcogenides. The elastic characteristics of this group of materials is quite similar to those of Cd and Zn chalcogenides.

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The stable crystalline phase of mercury sulphide is α-HgS (cinnabar structure). Zinc blende mercury sulphide (β-HgS) is an interesting modification of this II–VI compound (β-HgS is a narrow gap semiconductor with the inverted band structure). Due to the high free carrier concentration this crystal is considered as a suitable material for ohmic contacts for the wide-gap II–VI quantum structures. Recently this compound was also applied for growing the quantum dots (in CdS/HgS/CdS system). Nevertheless, the precise values of various physical parameters are still lacking in the literature for this semiconductor. In particular there exists only very limited information about the elastic properties of this material (which could be important from the point of view of possible future applications). Pure β-HgS can be obtained only by the non-equilibrium growth technique (usually in the form of thin layers etc.), therefore the possibility of the direct measurements of their elastic properties was highly limited in the past.

In the last few years the new method of bulk big size β-HgS crystal growth has been developed in the Institute of Physics of the Polish Academy of Sciences in Warsaw [1]. This method is based on zinc blende crystal structure stabilisation by HgS doping with the transition metal. The β-HgS crystals containing up to a few percent of Mn, Fe, or Co were obtained.

In some cases selected properties of doped material are very similar to the properties of pure compound. This is also the case of elastic constant values. Taking into account the fact that it is not possible to grow good quality big size monocrystals of pure β-HgS we decided to investigate the elastic properties of materials doped with the transition metal. Probably the most interesting compound was β-HgS doped with iron due to expected resonance character of this impurity in the semiconductor under discussion (for the details see [2]).

The present paper reports the results of the ultrasonic measurements performed at room temperature on samples prepared from highly Fe doped HgS monocrystals. The crystal orientation and the chemical composition of samples were determined by the X-ray diffraction. Each specimen was lapped and carefully polished in order to obtain a very flat surface, typical length of the crystal used for the measurements was equal to about 5 mm. Because of the cubic symmetry, the three adiabatic elastic constants of investigated compound are simply related to the acoustic velocities in the various crystallographic directions. These velocities (of both longitudinal and transverse waves) were measured by using the pulse-echo technique. Short pulses of 227 or 229 MHz acoustic waves were introduced into the sample. The transducer used both as an acoustic wave source and as a detector was separated from the sample by the crystalline quartz plate. The repetition time was equal to 20 μs. Pulses reflected from both an interface quartz/sample and from the opposite sample face came back to the detector giving rise to the narrow peaks observed in the experiment. The time delay between the sent pulse and different echoes arriving to the detector depends on the particular distance passed by the wave and the velocity of such wave in a given medium. Multichannel detection (10 ns per channel) was applied in order to separate the subsequent echoes. The amplitude of detected signal depends on the attenuation of the acoustic wave in the medium (such attenuation is higher for the investigated sample than that corresponding to the crystalline quartz).
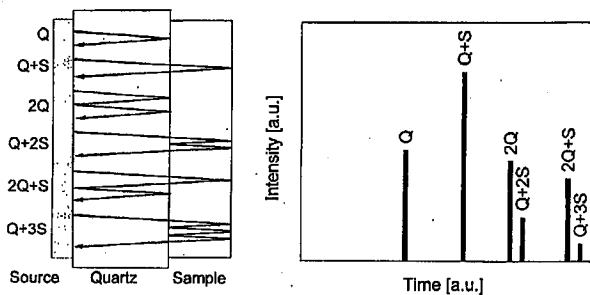

Fig. 1. An idea of the experiment. On the left: scheme of the sample support. Letters Q and S denote quartz and sample, respectively, and indicate how many times the acoustic wave passed through the particular medium before coming back to the detector. On the right: echoes spectrum expected for the investigated system, differences in the intensities are due to various wave attenuation in the sample and quartz.
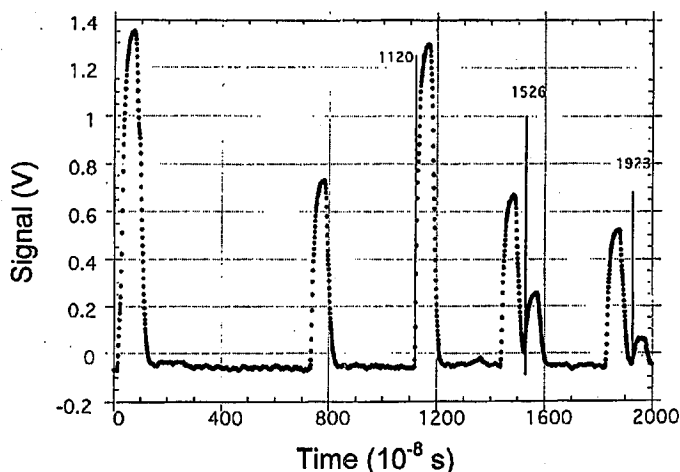
Fig. 2. An example of the experimental spectrum corresponding to the transverse wave propagation along [100] direction (room temperature data).

TABLE

Elastic constant values (given at 10^{10} N m^{-2} units) determined for zinc blende mercury chalcogenides.

Compound	c_{11}	c_{12}	c_{44}	Comments
HgTe	5.361	3.660	2.123	[7], room temperature
	5.971	4.154	2.241	[7], extrapolation to $T = 0$ K
HgSe	5.950	4.307	2.2015	[8], room temperature
	6.893	5.101	2.3069	[8], $T = 10$ K
	6.90	5.19	2.33	[6], extrapolation to $T = 0$ K
β-HgS	6.75	5.186	2.42	room temperature, this work
	7.53	–	2.28	[4, 5], neutron scattering, $T = 19$ K
	8.13	6.22	2.64	[3], low temperature theoretical predictions

An idea of the experiment is schematically shown in Fig. 1. The typical experimental result obtained for the propagation of the transverse waves along [100] direction is shown in Fig. 2. The first peak corresponds to the initial pulse, a few echoes can be observed before the next pulse is sent after 20 μs. The room temperature values of three elastic constants determined from the velocity of waves for β-HgS are given in Table. They are compared with the results of estimations given in the literature [3] as well as with the results of our previous measurements performed by means of inelastic neutron scattering [4, 5]. Selected experimental results obtained for other mercury chalcogenides are also shown for comparison [6–8]. As it is well known, the elastic constant values obtained from the slope of the acoustic

phonon branches given by the neutron scattering are determined with an accuracy much lower than those given by direct ultrasonic wave velocity measurements. From the comparison of the data given in Table well pronounced trend in the dependence of the elastic constant value on the anion in the mercury chalcogenide can be seen. The values of c_{11} and c_{12} clearly increase with an increasing ionicity of investigated compound (this ionicity is the highest for HgS and the smallest for HgTe). In the case of c_{44} elastic constant the differences between the values corresponding to different compounds are much smaller but the trend mentioned above is still seen. As expected, the room temperature values of elastic constants are smaller than those corresponding to low temperatures. Similar trends have been observed previously for other metal chalcogenides (Cd and Zn compounds — see, e.g. [9]). It should be stressed that due to the difference in the atomic mass of cations in various metal chalcogenides (and noticeably higher ionicity for all mercury chalcogenides in comparison to, e.g., Zn compounds) the absolute values of elastic constants are different for each group of materials.

As it was mentioned previously, one can expect that the elastic constants should be in practice the same for pure and doped β-HgS crystals. However, for the particular purposes an influence of the free carrier concentration on the elastic constants in zero-gap semiconductors have to be taken into account, as it was reported, e.g., for the case of HgTe [10]. Such contribution has been neglected in our case because according to the results of electron transport measurements the free carrier concentration for the samples under investigation does not exceed a value $n = 5 \times 10^{18}$ cm^{-3} (and the carrier related contribution to the elastic constants is negligible in this case).

In conclusion on the basis of the present data one can assume that (at least at room temperature) there is no anomaly in the elastic properties of β-HgS in comparison to, e.g., ZnS or CdS. Thus, zinc blende mercury sulphide can be considered as a potential candidate for growing II–VI quantum structures and devices. The general discussion of the elastic constant values for mercury chalcogenides will be possible when the ultrasonic experiments for β-HgS are performed also at low temperatures. Such measurements are in progress and their results will be soon available.

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