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High Resolution Infrared Spectroscopy of Phonons in the II-VI Alloys — The Temperature Dependencies Study

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Additional information is available at the end of the chapter

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1. Introduction

The cubic II-VI systems HgTe, CdTe and ZnTe are extremely interesting technologically materials with many applications such as infrared as well as quantum electronics devices [21, 29, 5, 44; 26]. The phonon frequencies of these alloys belong to the far-infrared region and investigation of their phonon spectra was one of more important problem in the infrared spectroscopy during 70-th years. The temperature dependence of the phonon HgTe-mode frequencies in binary HgTe, ternary HgCdTe (MCT) and HgZnTe (MZT) materials has been the subject of an intense debate in the last three decades [16, 14, 2, 1, 29, 4; Kozyrev et al., 1996; 31, 12, 35, 28], due to contradictory results regarding in particular the abnormal temperature shift of the HgTe-like TO-phonon frequency. The latter is opposite to the normal phonon frequency temperature shift of many alkali compounds as well as most of semiconductors. In fact, the HgTe-like TO-phonon frequency increases when temperature increases while the normal temperature shift associated with a crystal lattice expansion, has to be opposite: the frequency decreases when temperature is raised.

The different behaviour has been qualitatively explained by an electron-phonon (e - p) interaction contribution in work of [29] as the e - p -interaction would produce positive frequency shifts as the temperature is raised whose magnitude would exceed the negative shifts due to anharmonicity. However, the claiming that the e - p -coupling in the temperature shift of the optical phonon modes has a significant role should be better and quantitatively verified.

The e - p interaction is the main mechanism of charge carriers scattering in semiconductor crystals and low-dimensional structures together with impurities and defects. Particularly, the scattering on long wave longitudinal optical ($LO(\Gamma)$) phonons have an universal character because the latter generates a macroscopic polarized pole, and electrons experience very

effective interaction. Several resonance effects also occur such as the pinning of magneto-optical inter-band transitions observed in InSb by Johnson and Larsen (Johnson & Larsen, 1966). They affect the energy spectrum of electrons via the interaction with LO(Γ)-phonons. Effects produced by the direct polarized e-p-interaction, i.e., phonons affect the electron energy spectrum, are described in few review articles and books [22, 13]. In addition, the role of effects due to a direct non-linear polarized e-p-interaction has been shown in [32, 33].

On the other hand, reverse effects, i.e., how light electrons affect the phonon spectrum are much less known. Recently, we have shown [35] that the singularity in an electron energy spectrum induces a discontinuity in the phonon frequency temperature dependence of the $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ alloys. That means the appearance of an unexpected effect of strong resonance influence on oscillations of heavy atoms by the electron subsystem. In our short communication [36] we called this effect as returnable e-p interaction. It was shown that even though the returnable e-p-coupling has a non-polarized character, yet a deformation mechanism takes place [35, 36, 19]. It is necessary to note that singularity in the electron spectrum that induced the resonance returnable e-p interaction, is point of total zero of energy gap ($E_g \equiv \Gamma_6 - \Gamma_8 = 0$) well known in the $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ alloys (Dornhaus & Nimtz, 1985) and called later as a Dirac point.

It is then important to test the occurrence of this or similar effects in other semiconductor compounds. Moreover, it seems that the abnormal temperature dependence of the HgTe-like phonon modes can be solved in this framework, because the presence of a returnable e-p interaction could explain the positive temperature shift of the optical phonon frequencies. On the other hand, the positive temperature shift of the phonon frequency is characteristic for the HgTe-like modes in different Hg-based alloys such as the abovementioned HgCdTe , the HgCdSe [40, 39] and the HgZnTe as shown in the sequel. Data suggest that a spin-orbit relativistic contribution, larger for heavy atoms, play an important role in this phenomenon because of its effect on the chemical bond [42,17, 30].

The aim of this contribution is to generalize experimental data on the temperature dependence of the TO-phonon modes in the $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ and $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$ alloys of different compositions and analyze the influence of the resonance returnable e-p-interaction in case when the temperatures are close to singular Dirac point ($E_g \equiv \Gamma_6 - \Gamma_8 = 0$) and far from this point for alloys where the Dirac point exists. Such analyses should be performed on a background of obligatory anharmonic contribution caused by the temperature extension of the crystal lattice. That analyses should be distributed on the alloy compositions where the Dirac point exists not, also.

The rich experimental reflectivity data in the far IR region of MCT and MZT alloys that were collected during 2002-2006 years for different compositions and in a wide temperature range using a synchrotron radiation source [34, 27, Cebulski et al., 2008; 35, 36, 28] allow unique opportunity for such investigation.

2. Experiment

In order to investigate the temperature behaviour of the phonon modes for HgZnTe and HgCdTe alloys, several optical reflectivity measurements were performed in the far-IR region

at the DAΦNE-light laboratory at Laboratori Nazionale di Frascati (Italy) using a synchrotron radiation source (details on the experimental set-up are available in work(Cestelli Guidi et al., 2005)). A BRUKER Equinox 55 FT-IR interferometer modified to collect spectra in vacuum, was used. As IR sources both the synchrotron radiation from the DAΦNE storage ring and a mercury lamp were used. Measurements were performed from 20 to 300 K and in the wave-number range 50-600 cm^{-1} . In order to provide the spectral resolution of 1 cm^{-1} (2 cm^{-1} in some cases), we typically collected 200 scans within 600 s of acquisition time with a bolometer cooled to 4.2 K. The reflectivity was measured using as a reference a gold film evaporated onto the surface of the investigated samples. This method enabled us to measure the reflectivity coefficient $R(\omega, T)$ with an accuracy of 0.2%. The

$\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ crystals were grown at the Institute of Physics of the Polish Academy of Sciences in Warsaw (Poland) while the $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$ ones at the CNRS-Groupe d'Etude de la Matière Condensée (Meudon, France). The reflectivity curves $R(\omega, T)$ for $\text{Hg}_{0.90}\text{Zn}_{0.10}\text{Te}$ in the frequency range from 80 cm^{-1} to 220 cm^{-1} and in the temperature range 30-300 K are shown in Fig. 1.

Data show that the main phonon band consists of two subbands: a HgTe-like band in the range 118-135 cm^{-1} and a ZnTe-like band in the range of 160-180 cm^{-1} . Both of them are characterized by a fine structure. A non-monotonic temperature dependence of the reflectivity maxima can be also recognized. Similar $R(\omega, T)$ curves are showed in Fig.2 for the $\text{Hg}_{0.763}\text{Zn}_{0.237}\text{Te}$. The maxima on reflectivity curves in Fig. 2 are shifted with increase of temperature towards lower phonon frequencies monotonically.

To recognize the real frequency positions of a phonon mode, it is however necessary to calculate for each obtained experimental curve $R(\omega, T)$ the imaginary part of the dielectric function $\text{Im}[(\omega, T)]$ as function of frequency and temperature. That ones were calculated from the reflectivity spectra shown in Fig. 1 and 2 by means of the Kramers-Kronig (KK) procedure. This procedure is described in details in the work of [6]; was applied to experimental results presented in several papers, for example [35, 28, 25]. An estimated uncertainty of 1.5% takes place at calculation the $\text{Im}[(\omega, T)]$ curves for all experimental data. The $\text{Im}[(\omega, T)]$ curves at different temperatures are shown in Fig. 3 a,b for the $\text{Hg}_{0.90}\text{Zn}_{0.10}\text{Te}$ sample as well as in Fig. 4 a,b for the $\text{Hg}_{0.763}\text{Zn}_{0.237}\text{Te}$ sample. In Fig. 3 the $\text{Im}[(\omega, T)]$ -curves are presented separately for HgTe-band (Fig. 3a) and for ZnTe-band (Fig.3b).

It is necessary to underline here that the maximum of the HgTe-like sub-band (Fig. 3a) shifts towards higher frequencies when the temperature increases from 30 K to 80 K while at temperature higher than 85 K the maximum shifts to lower frequencies. A non-monotonic temperature dependence of the ZnTe-like sub-band (Fig. 3b) with maximum frequency position near 85 K is also observed.

The frequency positions of HgTe-like and ZnTe-like sub-band maxima determined from the $\text{Im}[(\omega, T)]$ curves at different temperatures in the range 30-300 K are shown for the sample $\text{Hg}_{0.90}\text{Zn}_{0.10}\text{Te}$ in Fig. 5a and 5b, respectively.

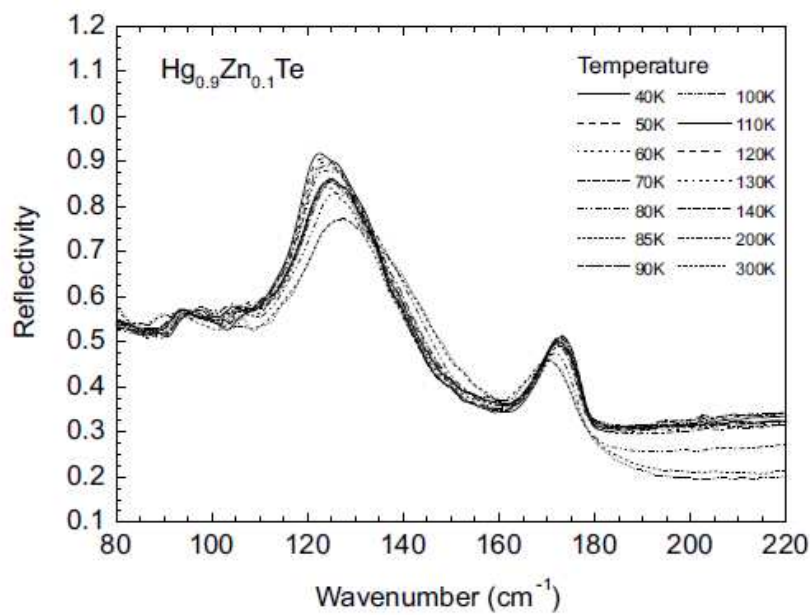


Figure 1. Reflectivity $R(\omega, T)$ for $\text{Hg}_{0.90}\text{Zn}_{0.10}\text{Te}$ in the frequency region from 80 cm^{-1} to 220 cm^{-1} and in the temperature interval 30 K-300 K

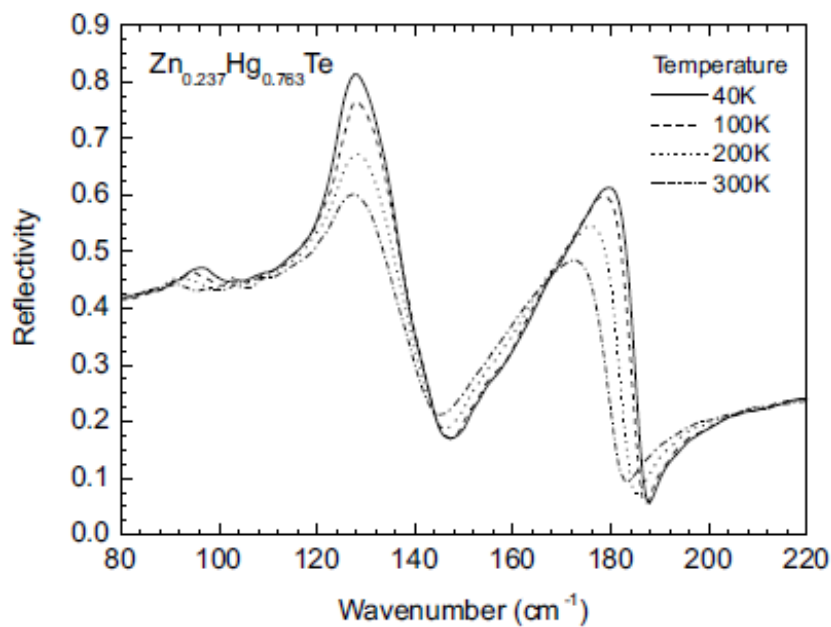


Figure 2. Reflectivity $R(\omega, T)$ for $\text{Hg}_{0.237}\text{Zn}_{0.763}\text{Te}$ in the frequency region from 80 cm^{-1} to 220 cm^{-1} and in the temperature interval 40 K-300 K

The KK-transformation was also performed for the $R(\omega, T)$ curves shown in Fig.2 (the $\text{Hg}_{0.763}\text{Zn}_{0.237}\text{Te}$ sample). The $\text{Im}[(\omega, T)]$ curves at different temperatures for this sample are shown

in Fig. 4, while the positions of the $\text{Im}[(\omega, T)]$ -maxima are shown in Fig. 6 a,b for the HgTe-like mode and the ZnTe-like mode, respectively.

Analogous investigations of the temperature dependence of the phonon frequencies for different modes were performed for another semiconductor alloy contained the mercury as one of component, namely: HgCdTe. The results were published earlier: [35, Sheregii et al. (2010), 28]. The measured curves of $R(\omega, T)$ for $\text{Hg}_{0.885}\text{Cd}_{0.115}\text{Te}$ in the frequency region from 80 cm^{-1} to 170 cm^{-1} and the temperature interval 40 K – 300 K are shown in Fig. 7. From Fig. 7 it is clearly seen, that the main phonon band consists of two subbands: a HgTe-like band in the range of $118\text{--}13\text{ cm}^{-1}$ and a CdTe-like band in the range of $140\text{--}160\text{ cm}^{-1}$ both characterized by a fine structure well known for the alloy phonon spectra [43, Kozyrev and Vodopynov 1996, 25]. A non-monotonic dependencies of the reflectivity maxima are seen too. The $\text{Im}[\varepsilon(\omega, T)]$ curves calculated from the reflectivity spectra are showed in Fig. 8 a,b. We have also to underline here that maximum of the HgTe-like sub-band is shifted towards higher frequencies when the temperature increases from 170 K to 240 K while for temperature higher than 240 K the maximum is shifted to lower frequencies. The similar temperature behaviour demonstrates the CdTe-like sub-band maximum.

The Verleur-Barker model [43] with five structural cells together with the statistical approach developed recently [26] is applied to the $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$ solid solutions. According to this model each of the two sub-bands: HgTe-like and ZnTe-like in the case of the $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$ alloys, consists of not more the four modes due to the oscillations of the Hg-Te or Zn-Te dipole pairs in each of the five tetrahedra T_n , where n is the number of Zn-atoms in the cell. Therefore, the maximum of each sub-bands can be associated to one of these four modes depending on the composition of alloy. In the case of the $\text{Hg}_{0.90}\text{Zn}_{0.10}\text{Te}$ alloy we combine the T_0 -mode with the HgTe-like sub-band and the T_1 -mode with the ZnTe-like mode, similarly to the $\text{Hg}_{0.85}\text{Cd}_{0.15}\text{Te}$ alloy. Regarding the $\text{Hg}_{0.763}\text{Zn}_{0.237}\text{Te}$ alloy the maximum of the HgTe-like sub-band is attributed to the T_1 -mode, while the maximum of the ZnTe-like subband, to the T_2 -mode. A comparison of the temperature dependence of the TO-mode frequencies showed in Fig. 3 and 6 point out a monotonic behaviour of the curves of the $\text{Hg}_{0.763}\text{Zn}_{0.237}\text{Te}$ sample (Fig. 6 a,b), while discontinuities occur in the curves of the semimetallic composition $\text{Hg}_{0.9}\text{Zn}_{0.1}\text{Te}$ (Fig. 4 and 5) with a positive temperature shift of the HgTe-like mode frequency and a negative temperature shift, for both compositions, of the ZnTe-like mode. In the sample $\text{Hg}_{0.763}\text{Zn}_{0.237}\text{Te}$ a similar temperature dependence of the HgTe-like and ZnTe-like TO-modes as in the sample $\text{Hg}_{0.80}\text{Cd}_{0.20}\text{Te}$ are observed the HgTe-like and CdTe-like TO-modes as shown in Fig. 10 a and b, respectively. For the sample $\text{Hg}_{0.763}\text{Zn}_{0.237}\text{Te}$, the frequency of the HgTe-like mode is practically independent of the temperature.

In Fig. 9 are shown the frequency positions of the HgTe-like and CdTe-like sub-band maxima on the $\text{Im}[\varepsilon(\omega, T)]$ curves for sample $\text{Hg}_{0.885}\text{Cd}_{0.115}\text{Te}$. It is seen from Fig. 9 that discontinuity is taken place precisely at 245 K for both HgTe- and CdTe modes. Generally, for CdTe-mode is observed negative temperature shift of the phonon frequency, while for HgTe-mode is positive one.

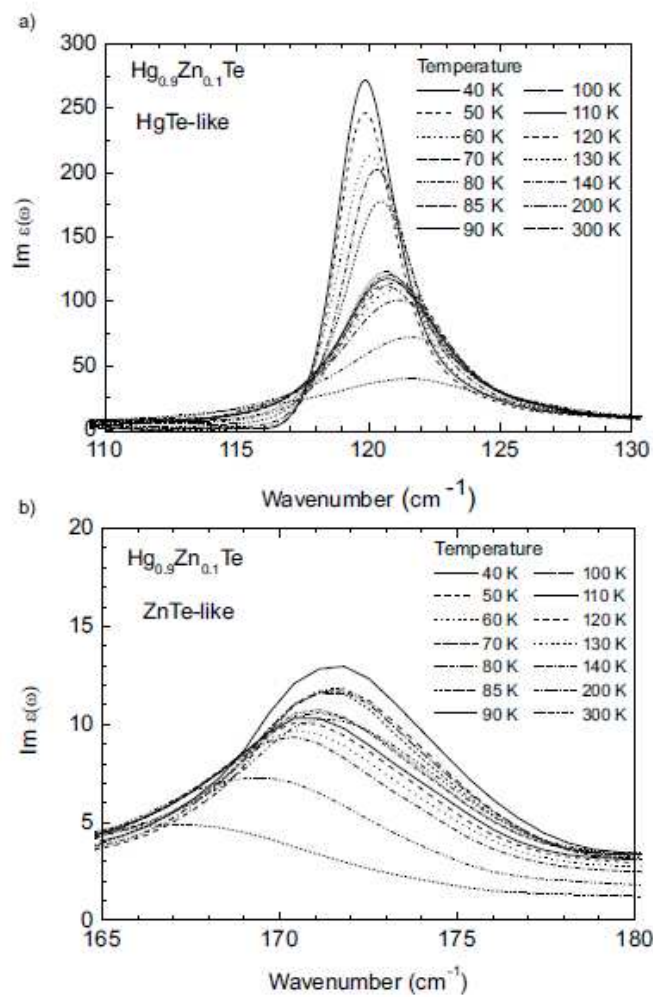


Figure 3. The $\text{Im}[(\omega, T)]$ curves of the $\text{Hg}_{0.90}\text{Zn}_{0.10}\text{Te}$ obtained from the reflectivity curves of Fig.1: a) the $\text{Im}[(\omega, T)]$ curves for the HgTe-like mode; b) the $\text{Im}[(\omega, T)]$ curves for the ZnTe-like mode.

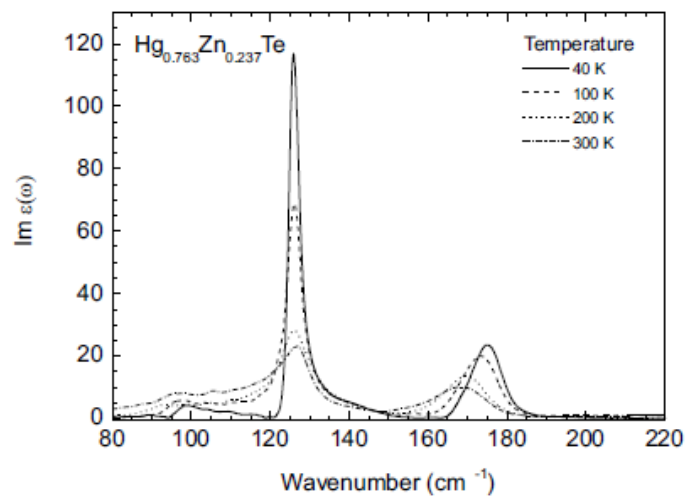


Figure 4. The $\text{Im}[\epsilon(\omega, T)]$ curves of the $\text{Hg}_{0.763}\text{Zn}_{0.237}\text{Te}$ obtained from the reflectivity curves of Fig.2.

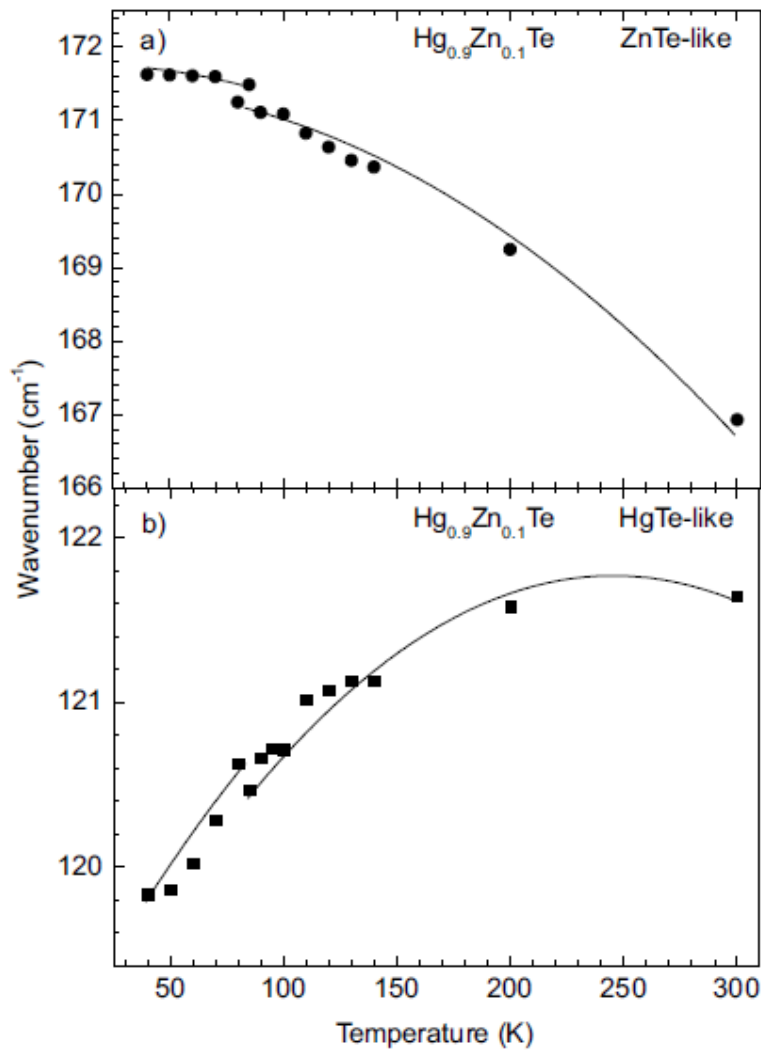


Figure 5. The frequency positions of ZnTe-like a) and HgTe-like b) sub-band maxima on the $\text{Im}[(\omega, T)]$ curves for the $\text{Hg}_{0.90}\text{Zn}_{0.10}\text{Te}$ at different temperatures in the range 30–300 K.

It is interesting to compare the temperature dependences of the phonon modes for another alloy of HgCdTe. As was shown in Fig. 6b for the sample $\text{Hg}_{0.763}\text{Zn}_{0.237}\text{Te}$, the frequency of the HgTe-like mode is practically independent of the temperature. Similar behaviour takes place for CdTe-mode in alloy $\text{Hg}_{0.80}\text{Cd}_{0.20}\text{Te}$ as it is seen in Fig. 10 where are shown the temperature dependences for the phonon mode frequencies for this alloy.

So, it is possible to generalise the obtained experimental results on temperature behaviour of the phonon spectra for four alloys containing mercury – $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$ and $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$. If composition x is near the value where the particularity in energy structure takes place, namely the Dirac point ($E_g \equiv \Gamma_6 - \Gamma_8 = 0$), for example in the case of the $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ alloys that is $x = 0.1 - 0.17$ and in the case of the $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$ alloys it is $x = 0.06 - 0.11$, then positive temperature shift is observed for the HgTe-modes with discontinuity the temperature where the Dirac point takes place.

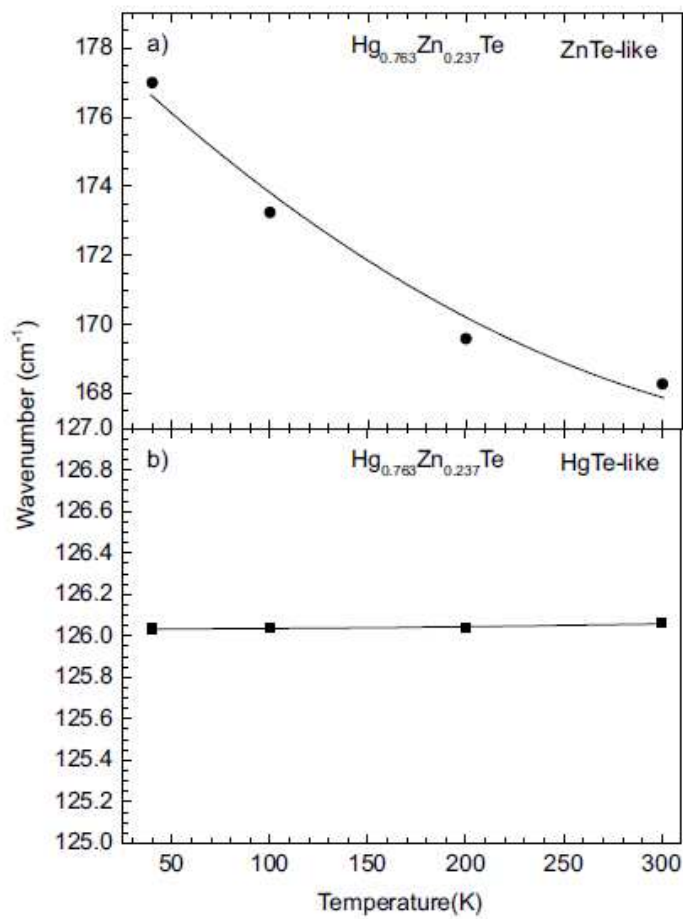


Figure 6. The positions of the $\text{Im}[(\omega, T)]$ -maxima for the $\text{Hg}_{0.763}\text{Zn}_{0.237}\text{Te}$ sample a) the ZnTe-like mode and b) the HgTe-like mode.

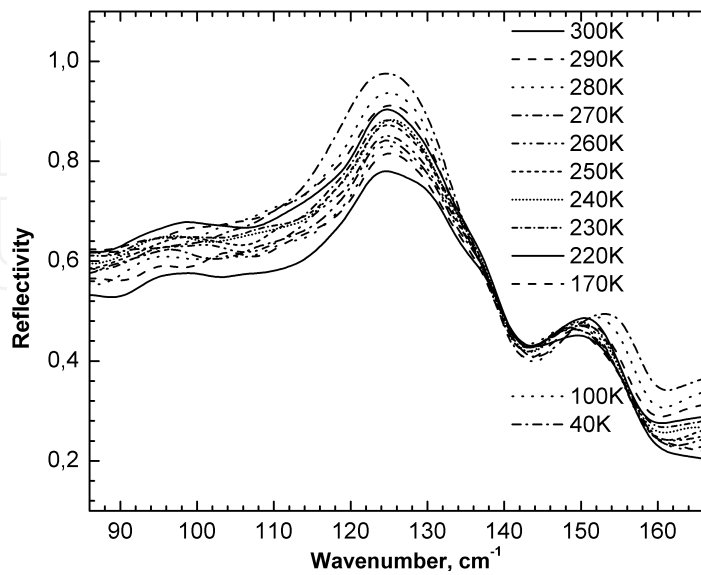


Figure 7. Reflectivity $R(\omega, T)$ for $\text{Hg}_{0.885}\text{Cd}_{0.115}\text{Te}$ in the frequency region from 80 cm⁻¹ to 220 cm⁻¹ and in the temperature interval 40 K-300 K

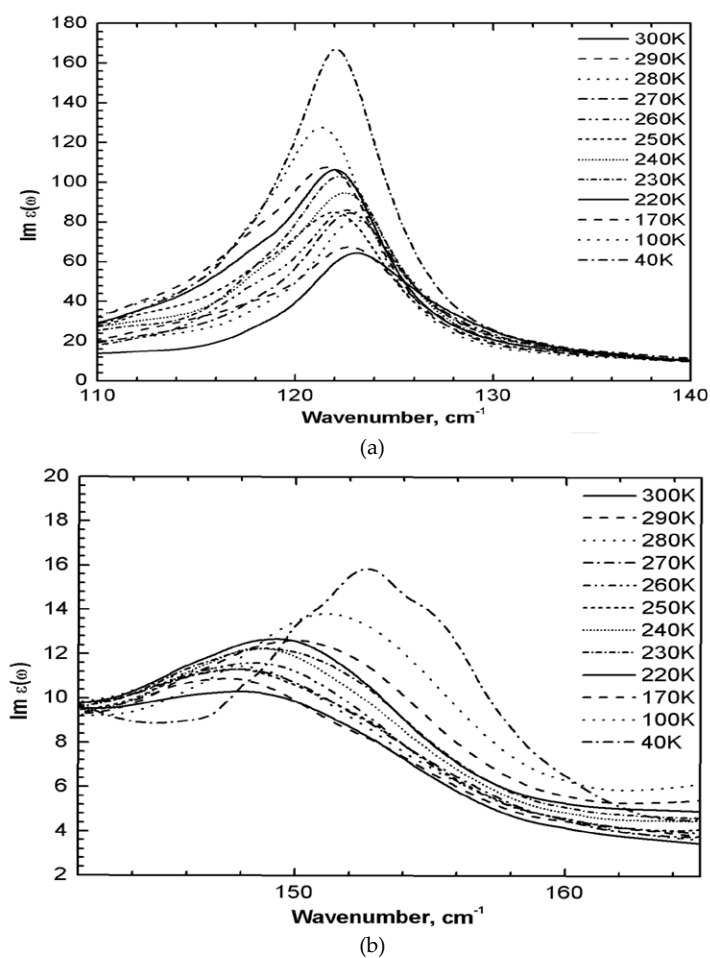


Figure 8. Reflectivity $R(\omega, T)$ for $\text{Hg}_{0.885}\text{Cd}_{0.115}\text{Te}$ in the frequency region from 80 cm^{-1} to 220 cm^{-1} and in the temperature interval 40 K-300 K

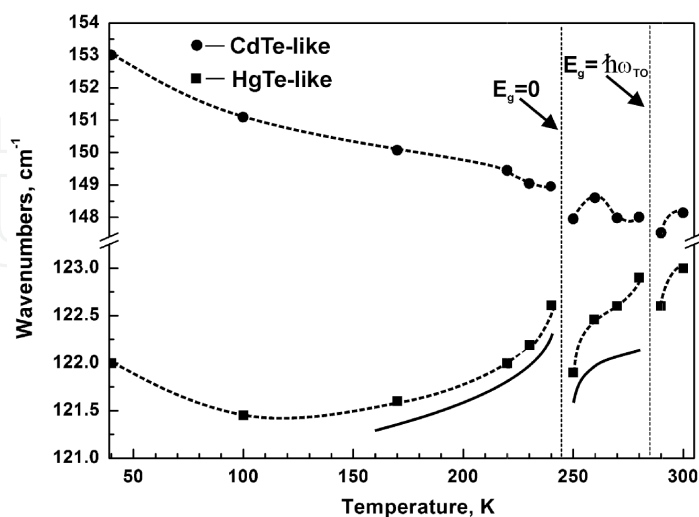


Figure 9. Reflectivity $R(\omega, T)$ for $\text{Hg}_{0.885}\text{Cd}_{0.115}\text{Te}$ in the frequency region from 80 cm^{-1} to 220 cm^{-1} and in the temperature interval 40 K-300 K

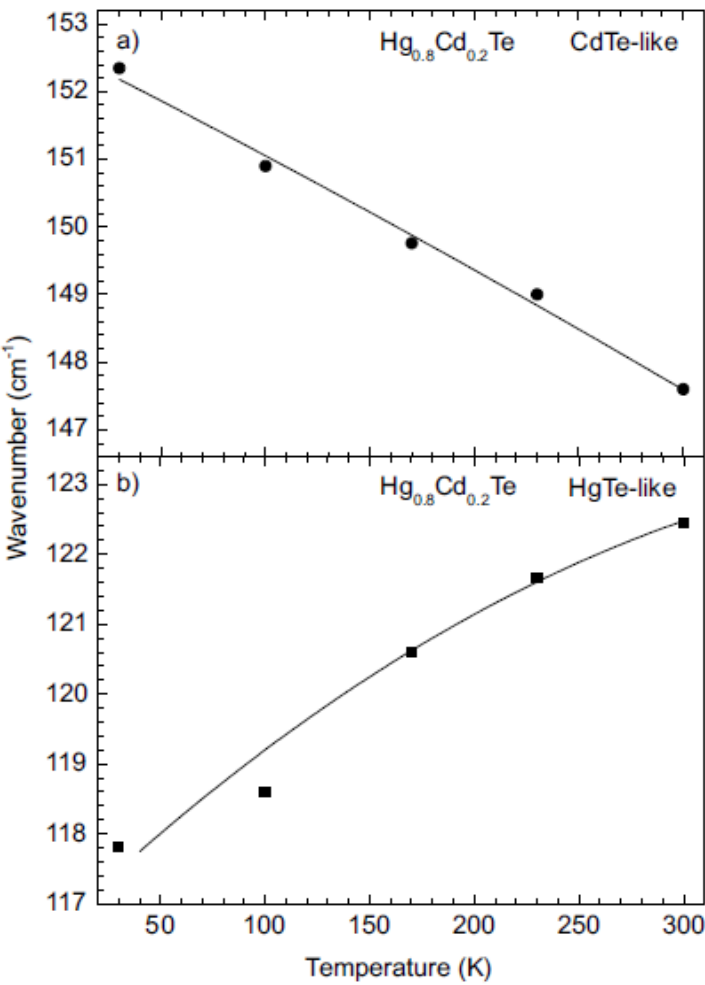


Figure 10. The positions of the $\text{Im}[(\omega, T)]$ -maxima for the $\text{Hg}_{0.80}\text{Cd}_{0.20}\text{Te}$ sample a) the CdTe-like mode and b) the HgTe-like mode.

Alloys	mode	A (cm^{-1})	B (cm^{-1})	C (cm^{-1})
$\text{Hg}_{0.85}\text{Cd}_{0.15}\text{Te}$	HgTe-like	121.8	-3.7	1.9
	CdTe-like	152.0	-2.3	-0.4
$\text{Hg}_{0.80}\text{Cd}_{0.20}\text{Te}$	HgTe-like	118.0	4	-0.6
	CdTe-like	152.4	-2	-0.4
$\text{Hg}_{0.90}\text{Zn}_{0.10}\text{Te}$	HgTe-like	119.2	3.6	-1.04
	ZnTe-like	171.2	-0.26	-1.87
$\text{Hg}_{0.763}\text{Zn}_{0.237}\text{Te}$	HgTe-like	126.03	0.001	0.005
	ZnTe-like	177.0	-10	2

Table 1. Parameters of alloys necessary to calculate the anharmonic contribution to the phonon frequency change

Alloy	W (eV)	Ξ_{CV} (meV)	A (Å)	E _F (meV)
Hg _{0.85} Cd _{0.15} Te	8	5	6.49	6
Hg _{0.80} Cd _{0.20} Te	8	5	6.49	1
Hg _{0.90} Zn _{0.10} Te	7	3	6.63	6
Hg _{0.763} Zn _{0.237} Te	7	3	6.65	1

Table 2. Parameters of alloys necessary to calculate the e-p contribution to the phonon frequency change

In the case of compositions apart from that areas where Dirac point could be presence (for $x > 0.17$ for Hg_{1-x}Cd_xTe alloys as well as for $x > 0.11$ for the Hg_{1-x}Zn_xTe alloys) an ambivalence behaviour for the temperature dependences of the HgTe-modes is observed – could be or strong positive temperature shift or complete independency on the temperature takes place.

3. Discussion

3.1. Basic theory

In view of the most general assumptions, it is possible to start from the following equation for the temperature shift of the TO_i-phonon mode frequencies ν_{TO_i} [18]:

$$\Delta \nu_{TO_i}(T) = \left(\frac{\partial \nu}{\partial T} \right)_P dT + \left(\frac{\partial \nu}{\partial T} \right)_V dT \quad (1)$$

The first term in Eq. (1) corresponds to the crystal expansion and to an anharmonic contribution to the harmonic crystal potential. This anharmonic term has been analyzed in detail by different authors in the last decades. The theory developed by Maradudin and Fein (Maradudin & Fein, 1962) as well as by [14] is based on the classical anharmonic oscillator. The potential energy is:

$$V(x) = cx^2 - gx^3 - fx^4 \quad (2)$$

where, the cubic term gx^3 gives a thermal expansion but no change in the frequency at the first order. The quartic term fx^4 and the cubic term to the second order $(gx^2)^2$ may induce a change in the frequency of the modes. The role of these terms was estimated [10] by assuming for Si atoms a covalent interatomic bond within the Morse potential:

$$V(r) = D[(e^{-a(r-r_0)} - 1)^2 - 1] \quad (3)$$

where the constants D , a and r_0 are determined, respectively, by bonding energy, stiffness of bond and interatomic spacing. Using the Morse potential to determine the coefficients of the Taylor series expansion of the potential, [14] find that the quartic term is positive, i.e., it increases with the frequency, but accounts for only 3/5 respect to the cubic term to the second order that is negative. The result is then a net decrease in the frequency.

In the quantum-mechanical approach each power of x correspond to a creation or an annihilation operator for a phonon, and the frequency shift of the optical mode is calculated as the self-energy of the mode [24]. Using this technique [10] performed detailed numerical calculations for the diamond structure using eigenvectors and eigenfrequencies of the harmonic model deduced by fitting the parameters of the dispersion curves obtained by inelastic neutron scattering data. The appropriate anharmonic interaction was determined by fitting experimental thermal expansion data. Later, Ipatova I.P. et al. (Ipatova et al., 1967) working on ionic crystals and Schall M. et. al. (Schall et al., 2001) in the CdTe and ZnTe semiconductors applied this theory to explain the temperature dependence of the dielectric function in the far IR frequency range.

The second term in equation (1) is due to the e-p interaction and it is interesting to underline that an analogue expression takes place for the temperature dependence of the energy gap in semiconductors (Yu & Cardona, 1996) where two contributions also occur: the anharmonic one and that induced by the e-p interaction.

3.1.1. Anharmonic contribution

An expression was derived by Ipatova I.P. et al. [16] for the temperature dependence of the phonon mode frequency ν_{TO} or the damping of an oscillator γ_{TO} in the quartic anharmonic force constant approximation:

$$Y(T) = A + B \left(\frac{T}{\Theta} \right) + C \left(\frac{T}{\Theta} \right)^2 \quad (4)$$

where $Y(T)$ is one of the measured quantities ν_{TO} or γ_{TO} , Θ is the characteristic temperature of the phonon subsystem $\Theta = h\nu_{TO} / k_B$ (k_B is the Boltzmann constant), A , B , C are the parameters obtained by fitting and for the CdTe phonon frequency (Ref. 12): $A=4.361$ THz (or 150 cm^{-1}), $B=-0.0298$ THz (or -1.00 cm^{-1}), $C=-0.0348$ THz (or -1.16 cm^{-1}). The same parameters for the ZnTe are: 5.409 THz (or 190 cm^{-1}), -0.0457 THz (or -1.52 cm^{-1}) and -0.0341 THz (or -1.37 cm^{-1}), respectively. In this case, it is clear that A is the frequency $\nu_{TO}(0)$ of the TO-phonon mode at $T=0$ and the first term in the equation (1) can be rewritten as:

$$\Delta \nu_{TO}^I(T) = B \left(\frac{T}{\Theta} \right) + C \left(\frac{T}{\Theta} \right)^2 \quad (5)$$

Because A and B are usually negative parameters, equation (5) always points out a frequency decrease, i.e., a softening of the phonon frequency on increasing the temperature. This behaviour has been observed in many ionic crystals and wide-gap semiconductors.

3.1.2. The e-p interaction contribution

As mentioned in the Introduction, the returnable e-p interaction could be responsible for the abnormal temperature dependence of the phonon frequency in both HgCdTe as well as HgZnTe. This kind of e-p interaction induces a discontinuity in the temperature dependence of the phonon frequencies in the resonant case, i.e., Dirac points. Actually, it is possible to assume that far from a Dirac point the returnable e-p interaction may overcome the anharmonic contribution and reverse the sign of the phonon frequency temperature dependence associated with the lattice dilatation.

As shown in [19], the preferred mechanism explaining the influence of the electronic structure of the crystal on its phonon spectrum is a deformation potential that mediates the interaction of electrons with the transverse optical phonons (TO-phonons). The TO-phonons are clearly recognized in optical reflectivity experiments, therefore the deformation potential is responsible for the interaction of electrons with TO-phonons. We are interested only in the terms of the deformation potential matrix that correspond to the energy region between the valence and the conduction band. Therefore, the self-energy of the TO-phonons with a small wave-vector q is given by the formula [19, 35]:

$$\omega_{TO}^{*2} = \omega_{TO}^2 - \int dE F(E) \left\{ \frac{1}{E + E_g + \hbar\omega_{TO}} + \frac{1}{E + E_g - \hbar\omega_{TO}} \right\} \quad (6)$$

where E_g is the energy gap and

$$F(E) = \frac{2}{2\pi^3} \int \frac{\omega_{TO}}{\hbar} \left(V_{cv}(k, q) \right)^2 \cdot \delta(E - E_c(k+q) - E_v(k)) dk \quad (7)$$

$V_{cv}(k, q)$ does not depend on the wave vector of the long-wave optical phonons ($q \rightarrow 0$); thus, $E_c(k+q) - E_v(k) = E_g$.

We can identify two kinds of singularities in Eq. (6): the first is obtained when E_g is equal to, and the second occurs when E_g equals zero. In the second case, if the temperature increases, the $E_g(T)$ dependence approaches zero from the negative side of the energy gap (the in-version band-structure). On the other hand, decreasing the temperature, the $E_g(T)$ dependence approaches zero from the positive side of the energy gap (normal band structure), hence, a discontinuity in $\omega_{TO}(T)$ may occur also at $E_g(T)=0$.

In order to describe the e-p contribution to the phonon frequency temperature dependence we may use an equation derived from Eq. (6) to determine the frequency change:

$$\omega_{TO}^{*2} = \omega_{TO}^2 \pm \frac{4\Xi_{CV}^2}{Ma^2W} \ln \frac{W}{2E_F + |E_g|} \quad (8)$$

where $\Xi(k, q)$ is the optical deformation potential, E_F is the Fermi energy measured from the band edge, W is the sum of the conduction and the valence bands width, a is the lattice constant and $E_g \equiv \Gamma_6 - \Gamma_8$ is the energy gap between the Γ_6 band, which is the conductive band in a normal semiconductor and the Γ_8 band, which is usually the top of the valence band. After a simple transformation from Eq. (8) we can obtain an expression for $\Delta\nu^{II}(T)$, the phonon frequency change associated to the returnable e-p interaction:

$$\Delta\nu^{II}(T) = \pm 2 \frac{\Xi_{CV}}{a} \sqrt{\frac{1}{MW} \ln \frac{W}{2E_F + |E_g|}} \quad (9)$$

Looking at $\Delta\nu^{II}(T)$ we may recognize the sign of this contribution through the corresponding sign of the deformation potential $\Xi(k, q)$: the sign is “-” when the energy gap ($E_g \equiv \Gamma_6 - \Gamma_8$) is positive (usually $E_g > 0$, in a normal semiconductor the deformation potential is negative) or the sign is “+” when $E_g < 0$ (that takes place before a Dirac point). Therefore, before the resonance case ($E_g \equiv \Gamma_6 - \Gamma_8 = 0$) when $E_g < 0$, $\Xi(k, q) > 0$ and the contribution of the returnable e-p interaction to the temperature change of the phonon frequency has a reversed sign with respect to the anharmonic contribution which is always negative. At some temperature a full reverse sign of the frequency could occur, i.e., when the phonon contribution overcomes the anharmonic one, on increasing the temperature also the frequency starts increasing. It enables us to explain the abnormal temperature dependence of the optical phonon frequency.

A different scenario occurs after the resonance: the sign is-for the phonon contribution to the temperature change of the phonon frequency when $\Xi(k, q) < 0$. The phonon frequency suddenly decreases and a discontinuity takes place at the Dirac point. However, on increasing the temperature the $E_g \equiv \Gamma_6 - \Gamma_8$ also increases, and the negative phonon contribution to the temperature change of the phonon frequency is reduced that implies a decrease of the negative change of this frequency. Therefore, the magnitude of the phonon frequency increases with the temperature after the Dirac point only if the phonon contribution overcomes the anharmonic one, a condition occurring not far from the resonance. As a consequence, the abnormal temperature dependence of the optical phonon frequency may occur also after the resonance.

3.1.3. Full temperature shift of the TO-phonon frequency

According to the above, the full temperature shift of the TO-phonon frequency in the semiconductor crystals is $\Delta\nu(T) = \Delta\nu^I(T) + \Delta\nu^{II}(T)$ (T) and the temperature dependence of the TO-phonon mode $\nu_{TO}(T)$ can be written as:

$$\nu(T) \equiv \nu_{TO}(0) + \Delta\nu_{TO}(T) = \nu_{TO}(0) + B\left(\frac{T}{\Theta}\right) + C\left(\frac{T}{\Theta}\right)^2 + 2\frac{\Xi_{cv}}{a} \sqrt{\frac{1}{MW} \ln \frac{W}{2E_F + (E_g)}} \quad (10)$$

From the comparisons of Eqns (5), (9) and (10) the anharmonic contribution exhibits for all crystals a monotonic function vs. temperature and, because the B and C constants are usually negative, the phonon frequency decreases (Ipatova et al., 1967; Schall et al., 2001). Actually, the e-p contribution depends dramatically on the temperature because $E_g(T)$ crosses through a point where $E_g=0$. In this point a singularity occurs and, because the e-p contribution is huge, a discontinuity in the temperature dependence of the phonon mode frequency is observed for $\text{Hg}_{0.89}\text{Cd}_{0.11}\text{Te}$ at 245 K (Sheregii et al., 2009). When $E_g < 0$, the $\Delta\nu^{\text{II}}(T)$ is positive and leads to the hardening of the phonon mode with increase of temperature. However, this contribution quickly reduces decreasing the temperature. Indeed, when temperature decrease the value of $|E_g|$ increases and $\Delta\nu^{\text{II}}(T)$ becomes smaller than $\Delta\nu^{\text{I}}(T)$ what means a softening of the phonon mode at low temperatures. In the semiconductor case at ($E_g > 0$), the $\Delta\nu^{\text{II}}(T)$ is negative and $|\Delta\nu^{\text{II}}(T)| > |\Delta\nu^{\text{I}}(T)|$ is fulfilled, because at $E_g \sim 0$ the e-p contribution is large. However, the increase of $|E_g|$ when temperature increase, leads to a decrease of the total negative change of the phonon frequency that implies a positive temperature shift of the magnitude of the phonon mode frequency already observed in the $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ as well as in another mercury contained alloys. So, it seems to be possible to explain this positive temperature shift of the phonon frequency by the e-p contribution. Nevertheless, concerning the role of the returnable e-p coupling, it is necessary to carry out a reliable experimental test of the above theoretical assumptions on the temperature dependence of the phonon mode frequency.

In what follows, we will present the analysis of the experimental data which are described above. Data allow to answer if the returnable e-p coupling contribution is enough to explain the abnormal temperature dependence of the HgTe-like mode frequency in both MCT and MZT alloys.

3.2. Analyses and Interpretation of experimental results

3.2.1. Alloy $\text{Hg}_{0.85}\text{Cd}_{0.15}\text{Te}$

The analysis of the observed temperature dependence of the TO-phonon modes for these semimetallic and semiconductor alloys is based on Eq. (10).

In order to calculate the e-p contribution to the temperature shift according to Eqns.(9,10) we need to know the temperature dependence of the energy gap $E_g(T)$. An empirical formula for $E_g(x,T)$ is presented in (Sheregii et al., 2009) derived for the $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ alloy. According this empirical formula the Dirac point ($E_g \equiv \Gamma_6 - \Gamma_8=0$) takes place for sample $\text{Hg}_{0.85}\text{Cd}_{0.15}\text{Te}$ at temperature 245 K. In Table 1 values of other important parameters are presented such as the optical deformation potential $\Xi(k, T)$, the Fermi energy E_F , the sum of the conduction, and the valence bands width as well as the lattice constant a for the HgCdTe and HgZnTe alloys. The A, B and C parameters for the anharmonic contribution for each sample are listed in Table 2.

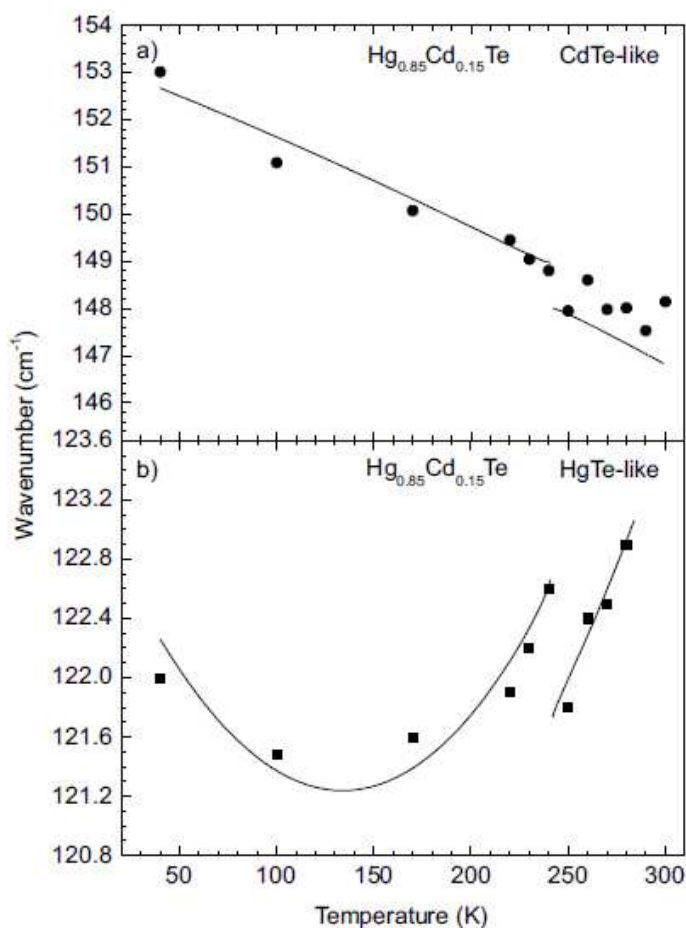


Figure 11. The CdTe-like (a) and HgTe-like (b) TO-mode positions in the frequency scale at different temperatures for the sample $\text{Hg}_{0.85}\text{Cd}_{0.15}\text{Te}$ – the same experimental points as in Fig. 9; solid curves are calculated according the Eqn. 10.

Result of the e - p contribution calculation according Eqn. (9) is shown by solid curve in Fig. 9. The discontinuity at 245 K is displayed by theoretical curve in narrow region of temperature very impressible and agree with experimental dependences very well. However, we need to confirm that Eq. (10) satisfactorily describes the experimentally observed temperature dependence of both HgTe-like and CdTe-like mode frequencies in wide temperature region together with the discontinuity observed at 245 K. Anharmonic and e - p terms in Eq. (10) match the experimental dependence of HgTe-mode in the whole temperature range from 40 K to 300 K for this sample as it is shown in Fig. 11b. The anharmonic contribution dominates at low temperature from 40 K to 120 K and the temperature shift of the HgTe-like T_0 -mode is negative. After the minimum at 121 K, the e - p -contribution overcomes the anharmonic one, and the HgTe-like T_0 -mode frequency start increasing up to resonance at 245 K. At the resonance (Dirac point) the e - p -contribution change sign and the phonon frequency suddenly decreases: the discontinuity takes place and the following increase of the temperature leads to a decrease of the negative e - p -contribution that induces the increase of the phonon frequency up to room temperature. It is important to note that theoretical curve in Fig. 11b is calculated with a positive value of the constant C . In the case of the CdTe-like mode (see Fig. 11a) both B and C

parameters are negative similarly to the CdTe-binary but the linear constant B is slightly larger than nonlinear while C is slightly smaller compared to the binary one. On the contrary, in the case of the HgTe-like mode it is impossible to have a satisfactorily theoretical agreement with experimental curves using negative values of both B and C constants. As a consequence, we take positive sign for the C constant what implies that *the thermal expansion can lead to an ambivalent effect in the frequency temperature dependence of the HgTe-like mode.*

3.2.2. Alloy $\text{Hg}_{0.80}\text{Cd}_{0.20}\text{Te}$

In the case of the $\text{Hg}_{0.80}\text{Cd}_{0.20}\text{Te}$ -alloy the singularity in the second term of Eq. (10) is very far (formally should exist at temperature closed to absolute zero) and the effect of the returnable e-p interaction is negligible. That is shown in Fig. 10b where we show experimental data and theoretical curves of the HgTe-like mode. Here the solid curve is calculated with the e-p term while the dotted one without it. Parameters are listed in Tables 1 and 2. A good fit of the experimental data was obtained with $B > 0$. It is clear from their behaviour that the phonon frequency of the HgTe-like mode strongly increases with the temperature, almost linearly, so that B must be large and positive.

The CdTe-like mode frequency has an opposite behavior vs. temperature with respect to the HgTe-like one: the frequency strongly decreases vs. temperature. It is a classical behavior where the anharmonic contribution dominates in the phonon frequency. The parameters B and C are close to that of the sample $\text{Hg}_{0.85}\text{Cd}_{0.15}\text{Te}$ and also of the binary CdTe.

3.2.3. Alloy $\text{Hg}_{0.90}\text{Zn}_{0.10}\text{Te}$

To calculate according to Eqns. (9, 10) the e-p contribution to the temperature shift of the temperature dependence of the energy gap $E_g(T)$ of the $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$, it is necessary to write an empirical formula $E_g(x, T)$ similar to that of the $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ (Talwar, 2010):

$$E_g(x, T) = -0.302 + 2.731x + 3.2410 - 2x - 0.629x^2 + 0.533x^3 + 5.310 - 4(0.76x^{0.5} - 1.29x)T \quad (11)$$

From the above equation calculated for the $\text{Hg}_{0.9}\text{Zn}_{0.1}\text{Te}$ and shown in Fig. 12, the zero-gap state should take place at 85 K.

Really, at this temperature 85 K a discontinuity of the temperature dependences of the HgTe-like and ZnTe-like modes is observed (see Fig. 5a and 5b). These discontinuities are smaller than in the $\text{Hg}_{0.85}\text{Cd}_{0.15}\text{Te}$ sample. In the case of the HgTe-like mode for the sample $\text{Hg}_{0.9}\text{Zn}_{0.1}\text{Te}$ (Fig. 5a), Eq. (10) describes quite well the experimental behavior with the discontinuity at 85 K but with a value $B=3.6$ which is positive that points out a strong increase of the phonon frequency with the temperature. So, the returnable e-p-interaction contribution in the second term in Eq. 10 describes the discontinuity in the phonon frequency temperature dependence but on top of a general increase of the frequency. A third factor, connected with the expansion but included not in Eqn. (10) openly, should cause this increase. The ZnTe-like mode temper-

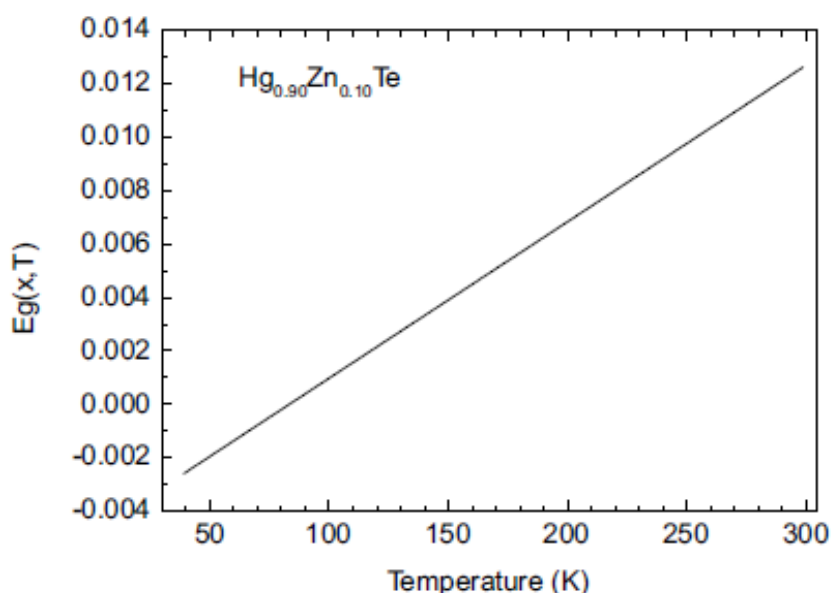


Figure 12. Temperature dependence of the energy gap ($E_g \equiv \Gamma_6 - \Gamma_8$) for the $\text{Hg}_{0.9}\text{Zn}_{0.1}\text{Te}$ alloy calculated according to the Eq.11 (see text).

ature behavior (Fig. 5b) can be interpreted by Eq.10 with the anharmonic constants $B=-0.26$ and $C=-1.87$ with a discontinuity always at 85 K.

3.2.4. Alloy $\text{Hg}_{0.237}\text{Zn}_{0.763}\text{Te}$

The sample $\text{Hg}_{0.763}\text{Zn}_{0.237}\text{Te}$ is characterized by the HgTe-like phonon frequency practically independent of the temperature as showed in Fig. 6b, and constants B and C close to zero. The $e-p$ contribution is then negligible similarly to the $\text{Hg}_{0.80}\text{Cd}_{0.20}\text{Te}$. Therefore, the two contributions are compensated in this system: one due to the anharmonicity that induces a negative frequency shift while the second, an unknown yet, induces positive temperature shift but the latter one is connected with thermal expansion too.

The temperature dependence of the ZnTe-like mode frequency in the case of the $\text{Hg}_{0.763}\text{Zn}_{0.237}\text{Te}$ alloy points out a maximal negative shift among all the alloys we investigated: $B=-10$ while $C=2$ is positive. The latter is due to the character of the mode frequency temperature dependence we observed. This character is different from the temperature dependence of the same mode for the $\text{Hg}_{0.90}\text{Zn}_{0.10}\text{Te}$ (Fig. 5a and 5b) as well as the CdTe-like TO-phonon frequency temperature dependence of both HgCdTe samples (Fig. 9 and 10a). In the binary ZnTe the temperature dependence of the ZnTe mode frequency is significantly smaller [14].

3.2.5. The relativistic contribution to vibrational effects

From the above data the positive temperature shift is characteristic in different alloys only of the HgTe-like modes. It means that contribution of Hg-atoms to the chemical bonds mainly affects the abnormal temperature dependence of the HgTe-like phonon frequencies. It is then

useful to consider the peculiarities of the chemical bonds in the case of the II-VI compounds with Hg.

Using a simple chemical picture of these compounds, Hg atoms contribute to bonds with two s electrons while Te atoms with two s and four p electrons. In comparison with Ca, Sr, and Ba chalcogenides, the ionicity of Hg chalcogenides is reduced. The Hg-d-electrons are partially delocalized, and, therefore, the effective nuclear charge, experienced by the valence electrons, increases. This generates a more tightly bound of Hg valence s electrons and, hence, a less ionic and more covalent bond. In this respect, Hg-atoms in the II-VI compounds are similar to the isoelectronic Cd and Zn in the same semiconductors. However, the d-shell delocalization is stronger in Hg than in Cd or Zn and, in fact, enough strong to pull the s level below the chalcogen p level¹⁰. As a consequence, an inverted band structure is obtained. The role of d-electrons in II-VI compounds is discussed in more detail by Wei and Zunger, [42], while the contribution of the spin-orbit interaction to chemical bonds and electronic structure is considered in [12]. This contribution increases with the number of atoms, and it is larger for Hg atoms with respect to Cd and Zn ones. In HgTe, the Γ_8 band is higher in energy than the Γ_6 one, whereas the situation is reversed in CdTe and ZnTe. Actually, this is because the energy difference between the Γ_8 and Γ_6 levels is determined by three factors: i) the chalcogen p-spin-orbit splitting, ii) the Hg-d-spin-orbit splitting and iii) the coupling strength among these states – so-called pd-coupling. For the p states, the Γ_8 symmetry is higher in energy than the Γ_7 , whereas for d-states the situation is reversed. Thus, if the p-spin-orbit coupling with the Hg-d-spin-orbit split states becomes reasonably small as in CdTe (ZnTe), the order of the Hg-d-spin-orbit split states drives the sequence order of Γ_8 and Γ_6 levels. Alternatively, if due to large pd-coupling the d character dominates in these bands, the Γ_8 level may also end up higher than the Γ_6 level.

However, how the difference between CdTe (ZnTe) and HgTe electronic structures translates into a temperature dependence of the phonon frequency? As it was underlined in the Subsection 3.1, a similar equation to Eq.(1) takes place for the temperature dependence of the energy gap in semiconductors where two contributions, the anharmonic one and that associated to e-p interaction, interplay with each other. It is interesting to note that the energy gap of HgCdTe and HgZnTe alloys have the same positive shift (Dornhaus & Nimtz, 1985) as the HgTe-like modes frequencies, actually opposite to the temperature shift observed for the energy gap of both CdTe and ZnTe [41, 23]. This difference in the $E_g(T)$ dependences for binary CdTe(ZnTe) and ternary HgCd(Zn)Te is due to the Hg-d-spin-orbit split states and, probably, is translated into the $\nu_{TO}(T)$ also due to a large pd-coupling of the chemical bonds. Although, the temperature dependence of the expansion coefficients in CdTe(ZnTe) and HgTe are similar (Bagot, 1993), the role of the lattice expansion on the $\nu_{TO}(T)$ dependences is different, similarly to the $E_g(T)$. It is possible to claim that the role of the quartic term in the potential of the Eq.(2) (see Subsection 3.1) is different for a Hg-Te bond compared to Cd-Te and Zn-Te ones because of the Hg-d-spin-orbit split states: overcomes others terms and positive temperature shift of the phonon frequency takes place.

4. Conclusion

It was performed an extensive experimental investigation of the temperature dependence of the phonon mode frequencies for Hg-based semiconductor alloys of II-VI compounds using the synchrotron radiation as a source in the far-infrared region. In the case of the $\text{Hg}_{0.9}\text{Zn}_{0.1}\text{Te}$ alloy we found a discontinuity of the temperature dependence of HgTe-like T0-mode and ZnTe-like T₁-mode similarly to the $\text{Hg}_{0.85}\text{Cd}_{0.15}\text{Te}$ alloy firstly found five years ago by [35]. A theoretical expression (Eqn. (10) in subsection 3.1) for the temperature shift of the phonon mode frequency has been derived including an anharmonic contribution as well as a term of a returnable electron-phonon interaction. It was shown that this expression including both abovementioned contributions satisfactorily describes the temperature shift of $\text{Hg}_{0.85}\text{Cd}_{0.15}\text{Te}$ and $\text{Hg}_{0.90}\text{Zn}_{0.10}\text{Te}$ alloys containing a Dirac point ($E_g \equiv \Gamma_6 - \Gamma_8 = 0$) if one of the two constants B and C describing the anharmonic shift of the HgTe-like mode, is positive. Moreover, in the case of the semiconductor alloys $\text{Hg}_{0.80}\text{Cd}_{0.20}\text{Te}$ and $\text{Hg}_{0.763}\text{Zn}_{0.237}\text{Te}$ the role of the returnable *e-p* contribution is negligible but a positive temperature shift for the HgTe-like modes takes place. The result cannot be explained as summing an *e-p* interaction as pointed out by (Rath et al., 1995).

The difference between the temperature behaviour of HgTe-like modes and CdTe-or ZnTe-like ones can be explained by the Hg-d-spin-orbit split contribution to the chemical bond. This contribution is responsible of the positive temperature shift of the energy gap of ternary HgCdTe and HgZnTe alloys with a narrow gap because the relativistic contribution to chemical bonds is also at the origin of the abnormal temperature shift of electron states in Hg-based semiconductors – inverse band structure. Similar effect is reasonably expected that the Hg-d-spin-orbit split contribution leads to an abnormal temperature shift of the HgTe-like phonon mode frequency.

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