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Deformation potentials of the semimetal HgTe

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It has been demonstrated that the hydrostatic deformation potential $C-a$ of a semimetal can be determined from the pressure dependence of intersubband transitions in superlattices containing the semimetal. By means of an investigation of optical absorption in $\mathrm{HgTe/Hg_{0.3}Cd_{0.7}Te}$ superlattices at hydrostatic pressures up to 3 GPa at room temperature the following values have been determined: $C-a=-3.69\pm0.10$ eV and $a^{\mathrm{HgTe}}-a^{\mathrm{CdTe}}=1.31\pm0.10$ eV, where C and a are the deformation potentials of the conduction and valence bands, respectively. Bulk HgTe normally undergoes a phase transition to the cinnabar structure at ≈1.3 GPa. However, this phase transition is frustrated in $\mathrm{HgTe/Hg_{0.3}Cd_{0.7}Te}$ superlattices and the HgTe layers are superpressed above 1.3 GPa.

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I. INTRODUCTION

The hydrostatic deformation potentials for the conduction and valence bands in a semiconductor, C and a, respectively, are important parameters; however, they cannot be directly determined experimentally. Their difference, $C-a$, can be determined from the hydrostatic pressure dependence of the band gap by means of excitonic absorption or photoluminescence.[1] Obviously this is not possible with a semimetal or many narrow-gap semiconductors. Nevertheless, in this article we shall demonstrate a direct method to determine the deformation potentials of either a semimetal or a narrow-gap semiconductor. In this method the hydrostatic pressure dependence of intersubband transitions in a superlattice or a multiple quantum well will be exploited.

As an example, type-III superlattices consisting of semimetallic HgTe and semiconducting $\mathrm{Hg_{1-x}Cd_xTe}$ layers will be considered in this article. The band structure and optical properties of these superlattices have been the subject of numerous investigations.[2] For moderately wide $\mathrm{Hg_{1-x}Cd_xTe}$ layers, it has been demonstrated that the band structure and the optical properties are primarily determined by the HgTe layer.[3] Consequently, this system offers a unique opportunity to investigate the band structure of semimetallic HgTe in a more direct manner. The nearly perfect match of the lattice constants makes this system ideal for such studies. Intersubband transitions in these superlattices have been investigated by means of optical absorption[2–4] and magnetoabsorption[5] experiments in conjunction with theoretical calculations. These intersubband transitions, and in particular the lowest energy gap, have also been linked to photoluminescence (PL) peaks in a number of investigations.[6]

Cheong *et al.*[7] have concluded that the hydrostatic pressure dependence of the observed PL peaks for a $\mathrm{HgTe/Hg_{1-x}Cd_xTe}$ superlattice is much less than that predicted by $\boldsymbol{k}\cdot\boldsymbol{p}$ band calculations based on the envelope function approximation (EFA). Their most prominent peak, which has been assigned to recombination across the SL band gap, has a pressure coefficient of ≤10 meV/GPa. However, their calculations employing the EFA with a range of reasonable SL parameters predict a pressure coefficient of at least ~65 meV/GPa for the band gap.

In contrast, the pressure dependence of the band gap of a number of semiconductors is in reasonable agreement with theoretical calculations.[8] More recent work has corroborated these results for II-VI semiconductors. In particular, this is true for CdTe whose experimental pressure dependence at pressures below 2 GPa lies between 79 and 83 meV/GPa at room temperature, independent of experimental method—i.e., a shift of either the absorption edge,[9] the corresponding PL peak,[10] or the reflectivity.[11] Values as low as 65 meV/GPa have been determined at 2–5 K for PL peaks involving excitons.[12,13] Furthermore, the pressure dependences of the PL peak energies in CdTe/ZnTe-stained layer superlattices[14] and $\mathrm{GaAs/Al_{0.32}Ga_{0.68}As}$ quantum wells[15] are comparable in magnitude to that of their constituents and are in good agreement with theoretical expectations.

In this investigation we have shown that the observed structure in transmission spectra of $\mathrm{HgTe/Hg_{0.3}Cd_{0.7}Te}$ superlattices which correspond to intersubband transitions does depend on pressure as is expected. More importantly, information concerning the hydrostatic deformation potentials of HgTe has been extracted from the pressure dependence of the intersubband transitions.

II. EXPERIMENTAL DETAILS

The two superlattices employed in this investigation were grown on $\mathrm{Cd_{0.96}Zn_{0.04}Te}(001)$ substrates in a Riber 2300 molecular beam epitaxial system at the University of Würzburg as has been described in detail elsewhere.[3] The thicknesses of the HgTe and $\mathrm{Hg_{0.3}Cd_{0.7}Te}$ layers were chosen such that the corresponding intersubband transitions were >280 meV in order to allow high-pressure transmission measurements in a diamond anvil cell. These measurements were carried out at the European laboratory for nonlinear spectroscopy (LENS) in Florence.

The samples were carefully polished, mechanically, and then chemomechanically, to a thickness of ~25–35 μm. No change in the transmission spectra was observed after polishing. They were then cleaved such that a nearly square sample with dimensions of $\sim 120 \times 120\ \mu\text{m}^2$ resulted. A sample together with a small ruby crystal, which was used to calibrate the pressure, was then loaded into a membrane diamond anvil cell from the Betsa company. Ar gas was employed as the pressure medium in the cell and hydrostatic pressure on the sample was generated by means of a membrane containing He gas. Type-IIa diamonds were employed which allowed transmission measurements to be carried out above an energy of 280 meV. The measurements were carried out using a Fourier transform spectrometer, Bruker HR-120, and additional components which have been described elsewhere.[16] The infrared radiation was focused onto the sample such that all light would have to pass through the sample.

III. THEORETICAL DETAILS

The absorption coefficient α and the transmission have been calculated using the envelope function method, as has been described in detail elsewhere.[3] The full 8×8 Kane Hamiltonian including all second-order terms representing the far-band contributions has been employed. A revised set of values for the band parameters deduced from measurements on bulk HgTe and $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ by Weiler[17] was employed which nevertheless reproduces the same bulk band structure at room temperature.

The Hamiltonian was modified according to Bir and Pikus[18] in order the include the influence of pressure in the model:

$$\Delta E_c(P) = C(x)3\epsilon(P), \tag{1}$$

$$\Delta E_v(P) = a(x)3\epsilon(P), \tag{2}$$

where $\Delta E_c(P)$ and $\Delta E_v(P)$ are the changes in the conduction and valence bands due to the hydrostatic pressure P, $C(x)$ and $a(x)$ are the deformation potentials of the conduction and valence bands,[19] and x is the Cd concentration of the layer in question. This was accomplished by using Murnaghan's equation of state[20]

$$\epsilon(P) = \frac{1}{3}\left[-1 + \left(1 + \frac{B_1}{B_0}P\right)^{-1/B_1}\right], \tag{3}$$

where B_0 is the bulk modulus and $B_1 = dB_0/dP$. The values of B_0 and B_1 for HgTe and CdTe employed in the model are listed in Table I. Both B_0 and B_1 are assumed to vary linearly with the composition x of the material in question. Consequently $\epsilon(P)$ is also a function of material composition.

IV. RESULTS AND DISCUSSION

In this investigation, the shift of intersubband transitions with hydrostatic pressure is of primary importance. This can be shown to be systematically correlated to the corresponding absorption edges in the smoothed transmission spectra shown in Fig. 1. The two steps correspond to the $H1$-$E1$ and $L1$-$E1$ intersubband transitions, where H, L, and E refer to heavy hole, light hole, and electron subbands, respectively. The band structure of this superlattice as well as these two intersubband transitions are shown in Fig. 2.

TABLE I. Summary of band gap pressure dependence, $C-a$, and strain parameters at room temperature. α calculated using Eq. (7) or (A3), β present investigation, and δ calculated using Eq. (A4).

Parameter	HgTe	Ref.	CdTe	Ref.
γ_0 (meV/GPa)	70–138[a]	23	79–83	9–11
B_0 (GPa)	42.3	24	42.50	25
B_1	3.78	26	4.20	25
$(C-a)$ (eV)	-4.4 ± 1.5	α	-3.42 ± 0.10	α
$(C-a)$ (eV)	-3.69 ± 0.10	β		
γ_0 (meV/GPa)	87.2 ± 2.5	α,β		
γ_1 (meV/GPa^2)	-4.61 ± 0.16	δ,β		

[a] At 4 and 77 K.

The presence of interference fringes shown in Fig. 1 due to the sample as well as to cavities between the sample and the diamond windows makes a determination of the absorption edge less precise. Therefore we have attempted to eliminate these interference fringes by taking the ratio of two transmission spectra at nearly the same pressure; see Fig. 3. The resulting extrema correspond to the transmission edges at the mean pressure if the pressure dependence is linear as is the case for small pressure differences. It can be easily shown that for a small shift in the transmission spectrum T,

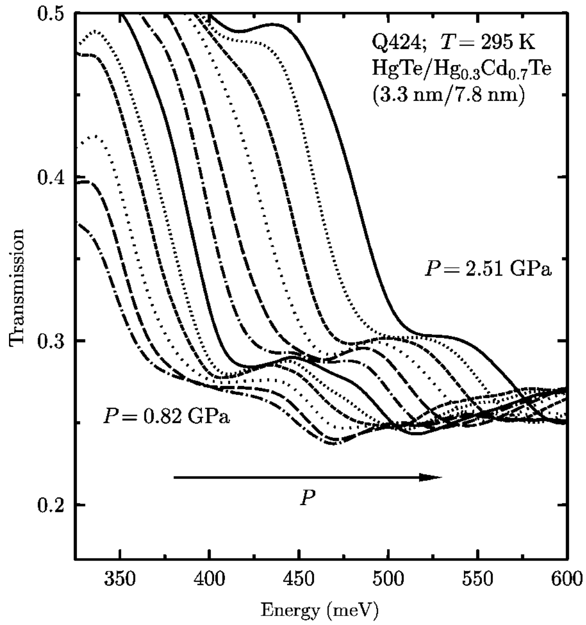

FIG. 1. Transmission spectra of Q424 at 295 K for pressures between 0.82 and 2.51 GPa. The two steps at lower and higher energies correspond to the $H1$-$E1$ and $L1$-$E1$ intersubband transitions, respectively.

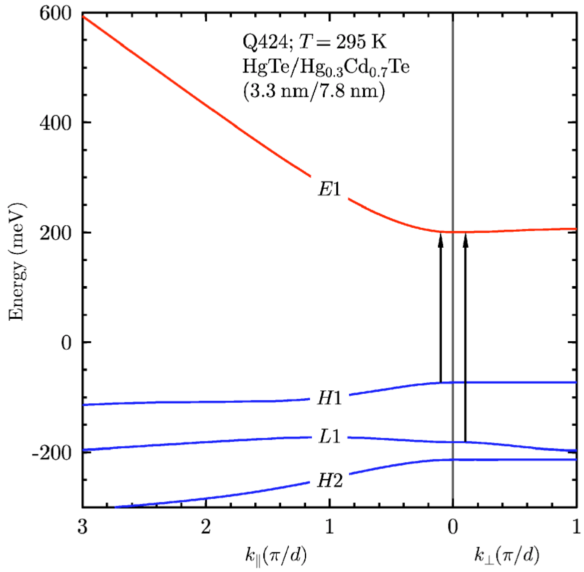

FIG. 2. The band structure of Q424 at 295 K and ambient pressure. The in-plane and perpendicular components of the wave vector, $k_{\parallel}$ and $k_{\perp}$, are in units of π/d where d is the superlattice period.

$$\frac{\Delta T}{T} \approx d\Delta\alpha, \tag{4}$$

where d and α are the thickness and absorption coefficient, respectively.

Obviously the resulting transmission ratio and $d\alpha/dE$ shown in Fig. 3 are in good agreement with experiment. In addition, the ratio of the amplitudes of the two maxima is in good agreement with the theoretically calculated ratio of the corresponding intersubband transitions—i.e., $H1$-$E1$ and $L1$-$E1$—see Fig. 3. Agreement for the amplitude ratio is good for all pressures with experimentally accessible transition energies—i.e., above 280 meV.

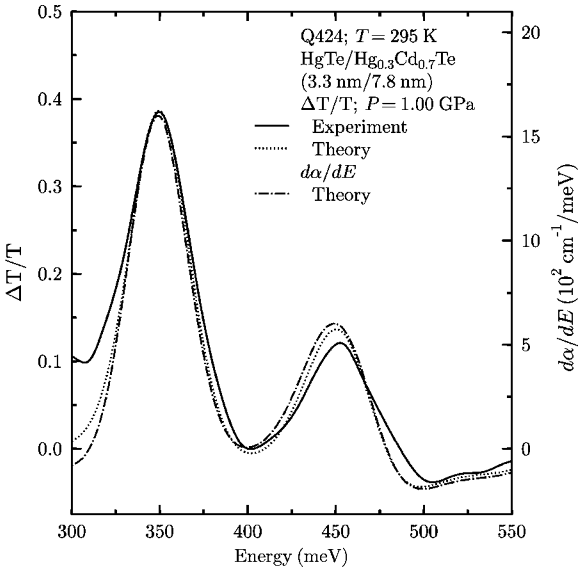

FIG. 3. Experimental and theoretical transmission spectra ratios ($T_{1.18\ \mathrm{GPa}}/T_{0.82\ \mathrm{GPa}}-1$), as well as $d\alpha/dE$ for Q424 at 295 K and a pressure of 1.00 GPa. The minima at lower and higher energies correspond to the $H1$-$E1$ and $L1$-$E1$ intersubband transitions, respectively.

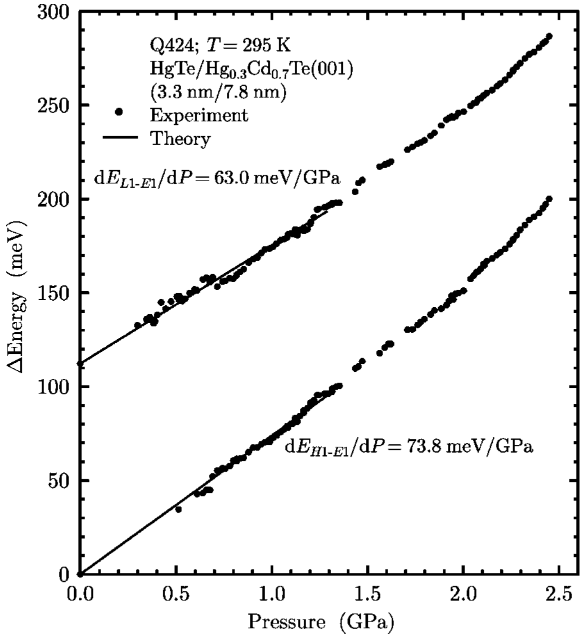

FIG. 4. Pressure dependences of the $H1$-$E1$ and $L1$-$E1$ intersubband transitions for Q424 at 295 K. The theoretical dependences according to the EFA calculations described in the text are indicated by solid lines up to the expected phase transition in HgTe at ~1.3 GPa.

Since dE_{i-f}/dP and not the absolute values of E_{i-f} are of interest, the theoretical and experimental intersubband transition energies as a function of pressure for Q424 have been normalized to the values at atmospheric pressure as is shown in Fig. 4. At pressures below 1.0 GPa, the slopes for $H1$-$E1$ and $L1$-$E1$ are 73.8 ± 1.0 and 63.0 ± 1.0 meV/GPa, respectively.

From the pressure dependence, knowledge of the conduction and valence band deformation potentials of HgTe and CdTe can be gained. $C(x)$ and $a(x)$ are assumed to vary linearly with the composition x of the Hg$_{1-x}$Cd$_x$Te layer. These parameters are related to the pressure dependence of the respective band gaps, dE_0/dP, according to

$$\frac{dE_0}{dP} = -(C-a)\frac{1}{B_0}. \tag{5}$$

Normally the pressure dependence of the band gap, E_0, of bulk materials is analyzed by means of a quadratic equation:

$$E_0(P) = E_0(0) + \gamma_0 P + \gamma_1 P^2. \tag{6}$$

Most authors either cite values of dE_0/dP assuming a linear dependence or determine γ_0 and γ_1 independently. However, it should be pointed out that γ_0 and γ_1 are not independent and γ_1 is not negligible. Frogley *et al.*[21] have advocated that the linear pressure coefficient should be defined and reported as dE_0/dP at zero pressure. However, in order to compare results from different materials it is necessary to use the ap-

TABLE II. Experimental and theoretical values of the pressure dependence of intersubband transition energies, dE_{i-f}/dP at 295 K.

	d_{HgTe}	d_{HgCdTe}	dE_{i-f}/dP (meV/GPa)			
	± 0.2	∓ 0.2	Experiment		Theory	
	(nm)	(nm)	$H1$-$E1$	$L1$-$E1$	$H1$-$E1$	$L1$-$E1$
Q230	3.1	7.5	71.5 ± 3.0	62.0 ± 3.0	74.3	63.8
Q424	3.3	7.8	73.8 ± 1.0	63.0 ± 1.0	73.8	63.0

propriate quadratic analysis since γ_0 and γ_1 are material dependent.

If higher terms of a Taylor expansion of Eq. (3) are neglected, then γ_0 and γ_1 are equal to

$$\gamma_0 = -(C-a)\frac{1}{B_0}, \qquad (7)$$

$$\gamma_1 = -\frac{1+B_1}{2B_0}\gamma_0. \qquad (8)$$

This normally leads to a very good approximation of the results of an analysis by means of Murnaghan's equation of state. Moreover, the values of γ_0 and γ_1 can be corrected, depending on the range of pressures over which the analysis is conducted. This is demonstrated in detail in the Appendix.

According to

$$\frac{\gamma_1}{\gamma_0} = -\frac{1+B_1}{2B_0}, \qquad (9)$$

$E(P)$ is always sublinear; however, in the present investigation $E(P)$ is hyperlinear above approximately 1.3 GPa. This coincides with the phase transition of HgTe from zinc blende to cinnabar.[22] Obviously this phase transition is suppressed by the superlattice, since no evidence for a phase transition is observed; $dE/dP(P)$ is a smooth function and no abrupt change in the experimental frequencies or relative amplitudes of the $H1$-$E1$ and $L1$-$E1$ intersubband transitions is observed.

Published values of dE_0/dP, or in most cases γ_0, for CdTe (Refs. 9–11) are reasonably consistent between 79 and 83 meV/GPa, whereas those for HgTe (Ref. 23) are not—i.e., 70–138 meV/GPa. The uncertainty in the HgTe values is compounded by the fact that they result from investigations of $Hg_{1-x}Cd_xTe$, not HgTe, and do not result from a direct measurement of a shift of the band gap. Moreover, even more uncertainty exists in individual deformation potentials C and a. Values for $C-a$ are summarized in Table I. To our knowledge, nothing has been published concerning $C-a$ for the $Hg_{0.3}Cd_{0.3}Te$ alloy. Therefore we have assumed that $C-a$ varies linearly with Cd concentration. $C-a$ for HgTe and $a^{\mathrm{HgTe}}-a^{\mathrm{CdTe}}$ have been used as the only adjustable parameters in the following calculations.

By fitting the experimental data, it has been shown that the pressure dependence of the $H1$-$E1$ and $H2$-$E2$ intersubband transitions depend on $(C-a)^{\mathrm{HgTe}}$ but are nearly independent of $(C-a)^{\mathrm{CdTe}}$:

$$\frac{dE_{H1-E1}}{dP} = f((C-a)^{\mathrm{HgTe}}) \qquad (10)$$

or

$$\frac{dE_{H2-E2}}{dP} = f((C-a)^{\mathrm{HgTe}}). \qquad (11)$$

The uncertainty in $C-a$ for CdTe given by 3.42 ± 0.10 eV results in a much smaller uncertainty in $C-a$ for HgTe expressed by 3.69 ± 0.02 eV. Furthermore, the difference in the pressure dependence between the $H1$-$E1$ and $L1$-$E1$ transitions depends directly on the difference in a between HgTe and CdTe,

$$\frac{dE_{H1-E1}}{dP} - \frac{dE_{L1-E1}}{dP} = f(a^{\mathrm{HgTe}} - a^{\mathrm{CdTe}}), \qquad (12)$$

and consequently on the pressure dependence of the valence band offset between HgTe and CdTe.

It should be mentioned here that other parameters including the $\boldsymbol{k}\cdot\boldsymbol{p}$ parameters do not significantly influence the calculated pressure dependence. The calculated values of dE_{i-f}/dP up to 1.0 GPa, which are listed in Table II and also plotted in Fig. 4, are in excellent agreement with the experimental values. This results directly in $C-a = -3.69 \pm 0.10$ eV for HgTe and $a^{\mathrm{HgTe}}-a^{\mathrm{CdTe}} = 1.31 \pm 0.10$ eV. These uncertainties are due to a combination of uncertainties in parameters taken from the literature and the experimental data.

Agreement between the calculated results and the experimental data for Q230 at 295 K is also good, even though the statistical significance of the data is less than that of Q424. Substitution of $C-a = -3.69 \pm 0.10$ eV into Eq. (7) results in $\gamma_0 = 87.2 \pm 2.5$ meV/GPa for HgTe.

The energy difference between the first heavy hole and the first light hole subbands is determined primarily by the valence band offset Λ between HgTe and CdTe.[3] Consequently, a difference in the pressure dependence of the $H1$-$E1$ and $L1$-$E1$ intersubband transitions is due to the pressure dependence of Λ. Because B_0 and B_1 are nearly equal for HgTe and CdTe—i.e., $\boldsymbol{\epsilon}^{\mathrm{HgTe}}(P) \approx \boldsymbol{\epsilon}^{\mathrm{CdTe}}(P)$—using Eqs. (2) and (3) its follows that

$$\Delta E_v^{\mathrm{HgTe}} - \Delta E_v^{\mathrm{CdTe}} = (a^{\mathrm{HgTe}} - a^{\mathrm{CdTe}})3\boldsymbol{\epsilon}^{\mathrm{CdTe}}(P), \qquad (13)$$

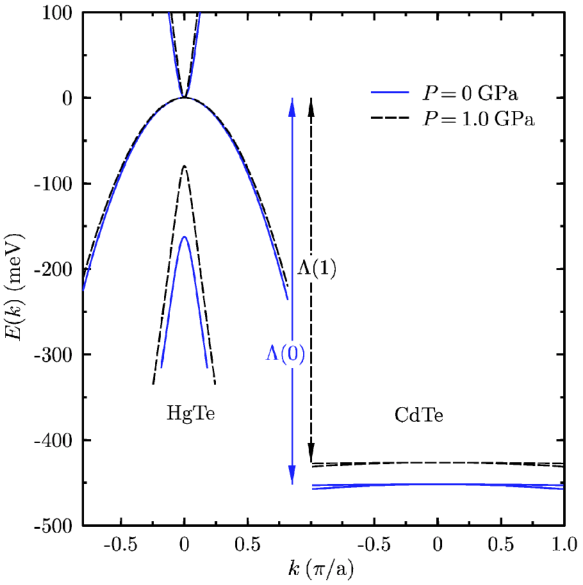

FIG. 5. The energy dispersion $E(\boldsymbol{k})$ of the light and heavy hole valence bands for HgTe and CdTe as well as the first conduction band for HgTe for two different pressures at 295 K. The dispersion of the CdTe valence bands is much flatter due to its larger hole effective masses. The valence band offset $\Lambda(P)$ at 0 and 1.0 GPa is indicated.

$$a^{\mathrm{HgTe}} - a^{\mathrm{CdTe}} \approx - B_0^{\mathrm{CdTe}} \frac{d\Lambda}{dP}. \tag{14}$$

It is note worthy that $d\Lambda/dP$, which is a heterostructure parameter, results from knowledge of the bulk parameters.

The calculated energy dispersion $E(\boldsymbol{k})$ of the light and heavy hole valence bands for HgTe and CdTe as well as the first conduction band for HgTe is shown in Fig. 5 for 0.0 and 1.0 GPa at room temperature. Due to the large heavy and light hole effective masses for CdTe, its valence band dispersion is very flat. In contrast the electron and light hole dispersion for HgTe, and even that of its heavy hole, is much more pronounced. The pressure dependence of Λ for $P \leqslant 1.0$ GPa at 300 K is indicated in Fig. 5 and is also given by

$$\Lambda(P) = \Lambda(0) + \frac{d\Lambda}{dP}P, \tag{15}$$

where $\Lambda(0) = 450$ meV according to Ref. 3 and $d\Lambda/dP = -25$ meV/GPa.

It should be pointed out that the intersubband transition pressure dependence, which is a salient feature of this investigation, is nearly independent of the values of the superlattice parameters over a wide range of values. For example, as shown in Fig. 6, an uncertainty in the HgTe width of ±0.5 nm leads to an error of merely ±0.10 eV in $C-a$ for HgTe as well as ±0.10 eV in $a^{\mathrm{HgTe}} - a^{\mathrm{CdTe}}$.

In addition, if the $H1$-$E1$ intersubband transition is below 280 meV and therefore not observable, then the pressure dependence of $H2$-$E2$ can be employed to determine $C-a$ according to Eq. (11).

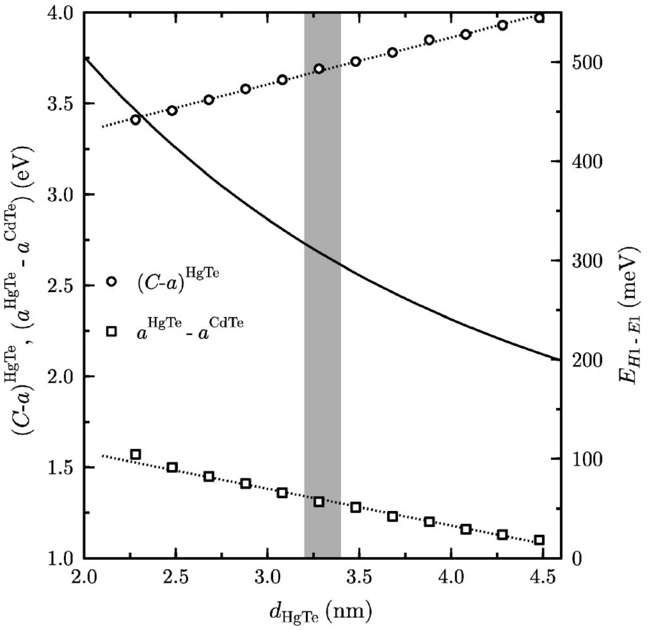

FIG. 6. Values of $(C-a)^{\mathrm{HgTe}}$ and $a^{\mathrm{HgTe}} - a^{\mathrm{CdTe}}$ versus the HgTe thickness, d_{HgTe}, necessary to reproduce the experimentally determined values of γ_0 for the $H1$-$E1$ and $L1$-$E1$ intersubband transitions for Q424 at 295 K. The dotted lines are merely guides to the eye. Values of $E_{H1\text{-}E1}$ versus d_{HgTe} are also plotted as a solid line. The long vertical gray area corresponds to the uncertainty in d_{HgTe}.

Only theoretical values or indirectly determined experimental values for either a^{HgTe} or a^{CdTe} have been published—for example, according to the tight-binding calculations of Merad *et al.*,[27] $a^{\mathrm{CdTe}} = 0.76$ eV. In addition, according to Takita and Landwehr,[28] $a^{\mathrm{HgTe}} = 3.8$ eV. This would require that $C \approx 0$. In other words, almost the entire pressure dependence would be due to a shift of the valence band and none to that of the conduction band. This is not the case for any other material to our knowledge. In all fairness, it should be mentioned that the results of Takita and Landwehr were obtained by means of a less direct method involving multiple phonons. Regardless of the individual values, the present method allows $a^{\mathrm{HgTe}} - a^{\mathrm{CdTe}}$ to be experimentally determined with excellent precision.

At pressures below 1.0 GPa, dE_{i-f}/dP for $H1$-$E1$ and $L1$-$E1$ with values of 73.8 ± 1.0 and 63.0 ± 1.0 meV/GPa, respectively, are in good agreement with theory as can be seen in Fig. 4. Above 1.3 GPa the experimental results can not be explained by our model. Bulk HgTe undergoes a phase transition from zinc blende to cinnabar at ~1.3 GPa.[22] However, there is no sharp change in the intersubband energies and no destructive change in the sample at pressures near 1.3 GPa. Moreover, the experimental results are reversible up to at least 2.5 GPa. Therefore it seems reasonable to suggest that the observed increase in dE_{i-f}/dP is due to a frustration of this phase transition. In other words, these thin HgTe layers are stabilized by the neighboring $Hg_{0.3}Cd_{0.7}Te$ layers; i.e., they are superpressed.

V. CONCLUSION

We conclude that the hydrostatic deformation potential, $C-a$, for a semimetal can be determined by means of the pressure dependence of intersubband transitions of a superlattice containing the semimetal. In addition a precise value of $a^{\mathrm{HgTe}}-a^{\mathrm{CdTe}}$ results from $dE_{H1\text{-}E1}/dP-dE_{L1\text{-}E1}/dP$. In this investigation $C-a=-3.69\pm0.10$ eV for HgTe and $a^{\mathrm{HgTe}}-a^{\mathrm{CdTe}}=1.31\pm0.10$ eV.

In contrast to the photoluminescence results of Cheong *et al.*,[7] we have shown that the observed structure in transmission spectra of HgTe/Hg$_{0.3}$Cd$_{0.7}$Te superlattices which correspond to intersubband transitions does depend on pressure as is expected. Furthermore, employment of this model results in the correct electronic band structure of HgTe/Hg$_{1-x}$Cd$_x$Te superlattices and the correct dependence on hydostatic pressure. Bulk HgTe normally undergoes a phase transition to the cinnabar structure at ≈1.3 GPa. However, this phase transition is frustrated in HgTe/Hg$_{0.3}$Cd$_{0.7}$Te superlattices and the HgTe layers are superpressed above 1.3 GPa.

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APPENDIX

If the equation

$$E_0(P)=E_0(0)+\gamma_0P+\gamma_1P^2 \tag{A1}$$

is considered to be the result of a least-squares fit of an equation involving Murnaghan's equation of state,[20] where higher terms are neglected, then the values of the coefficients γ_0 and γ_1 depend on the range of pressure involved in the analysis of the data. Assuming that range is given by

$$\frac{P}{P_m}\in[0,1],\quad \frac{B_1}{B_0}P_m\leqslant 1, \tag{A2}$$

then

$$\gamma_0=-(C-a)\frac{1}{B_0}(1-S_0), \tag{A3}$$

$$\gamma_1=-\left[\frac{1+B_1}{2B_0}(1-S_1)\right]\gamma_0, \tag{A4}$$

where

$$S_i=\frac{P_m}{B_0}\left[Z_{i1}+Z_{i2}B_1+(Z_{i3}+Z_{i4}B_1)\frac{P_m}{B_0}\right]. \tag{A5}$$

A least-squares analysis results in the values

$$Z_{01}=0.1182,\quad Z_{11}=0.9338,$$

$$Z_{02}=-0.0207,\quad Z_{12}=0.4850,$$

$$Z_{03}=-1.2677,\quad Z_{13}=0.1069,$$

$$Z_{04}=0.6235,\quad Z_{14}=-0.9101.$$

If P_m is sufficiently small, then $S_0\ll1$ and $S_1\ll1$, and Eqs. (A3) and (A4) reduce to the first two coefficients of a Taylor's expansion of Murnaghan's equation of state:

$$\gamma_0=-(C-a)\frac{1}{B_0}, \tag{A6}$$

$$\gamma_1=-\frac{1+B_1}{2B_0}\gamma_0. \tag{A7}$$

In this investigation P_m has been taken to be 1.0 GPa, and consequently $S_0\approx0.0016$ and $S_1\approx0.064$. Therefore only one of the two conditions—i.e., $S_0\ll1$—is fulfilled. The value of ≈0.064 for S_1 results in an approximately 6.4% smaller value of $|\gamma_1|$.

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