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Different temperature renormalizations for heavy and light-hole states of monolayer-thick heterostructures

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Abstract

We have found that the energy splitting between peaks in the linearly polarized emission from the cleaved surface of an InAs/GaAs monolayer structure triples with increasing temperature in the range from 5 to 150 K. For each polarization the main emission line corresponds to the radiative recombination of either heavy or light-hole excitons bound to the monolayer. The striking temperature behavior of the peak energies originates from the different hole–phonon coupling due to the much larger penetration of the light-hole envelope function into the GaAs. We prove this assertion by confining the light holes to the InAs plane with a strong magnetic field, which leads to a reduction of the temperature dependence of the heavy–light hole splitting.

Keywords: A. Quantum wells; D. Electron–phonon interactions; D. Thermal effects; E. Luminescence

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The electron–phonon interaction plays a key role in a variety of solid-state physical phenomena like superconductivity, electrical and thermal transport, light-scattering processes, among many others [1]. It is also at the origin of changes of the band structure of semiconductors with temperature [2–5] or isotopical substitution [6,7]. Electronic states are renormalized via their interaction with lattice vibrations leading to a reduction of direct band-gap energies with increasing temperature. For almost all tetrahedrally coordinated semiconductors [8–10] the temperature shift of band gaps is well described by the empirical relation [11]

$$E_g(T) = E_0 - \frac{\alpha_{ph}}{e^{\beta_{ph}/T} - 1}, \quad (1)$$

which is essentially given by a Bose–Einstein statistical factor for phonons with average frequency β_{ph}. The parameter α_{ph} is a measure of the strength of the gap renormalization by electron–phonon interaction and E_0 corresponds to the gap energy renormalized by zero-point vibrations. Experimentally, it is well established that near band-edge states like shallow defects and Wannier-type excitons [8–10], which are characterized by spatially delocalized wave functions, exhibit the temperature dependence of the band gap they are associated with. The same holds for optical transitions between confined electron and hole states in quantum well (QW) structures [12–15]. In all these cases, temperature effects are mainly determined by the coupling of the Bloch part of the wave function to bulk phonons.

Semiconductor heterostructures consisting of extremely thin InAs layers in bulk-like GaAs are among the best examples of a low-dimensional system where confinement energies are affected by the large built-in strain (~7%) [16–19] and by the penetration of the envelope function into the barrier material. InAs/GaAs monolayer (ML) structures have also attracted renewed attention due to their unusual lasing properties [20,21] and the close relation to self-organized quantum dots [22–24]. The reduced dimensionality of the structure manifests itself in the spectrum of vibrations as well. It exhibits several optical phonon modes tightly

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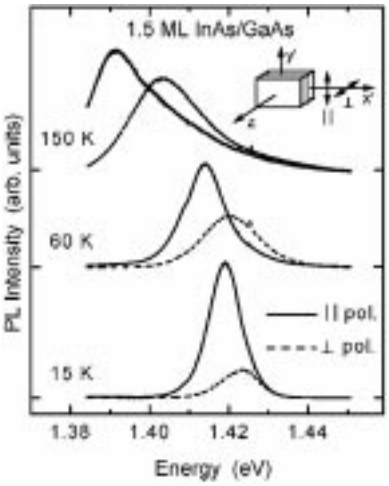

Fig. 1. Linearly polarized PL spectra of the 1.5 ML InAs/GaAs sample at different temperatures. The inset shows a sketch of the scattering geometry. The symbol ∥ (⊥) denotes, respectively, parallel (perpendicular) linear polarization of the emitted light with respect of the InAs plane.

confined to the InAs layer and energetically separated from the GaAs bulk modes [25]. An interesting question is whether low-dimensional systems characterized by strong quantum confinement show a phenomenology similar to bulk materials regarding the interplay between electronic and vibrational properties.

Here we report on the impact of the wave function extent on the electron–phonon interaction at the example of an InAs/GaAs monolayer structure revealed by the temperature variation of the polarized emission from a cleaved edge. With increasing temperature we observe a strong increase of the energy splitting between the emission peaks in each polarization corresponding to the recombination of bound heavy- and light-hole excitons. From experiments at high magnetic fields we are able to demonstrate that this temperature behavior arises from differences in the hole–phonon coupling. Whereas light holes couple with the bulk GaAs phonons, the heavy holes interact considerably with the softer modes confined to the InAs layer.

Samples correspond to the one used in the laser structure described elsewhere [20,21]. They consist of a single InAs layer (effective thickness about 1.5 ML) sandwiched between two 300 nm thick GaAs layers. Mirror-like surfaces perpendicular to the InAs ML were obtained by cleaving the sample. Photoluminescence (PL) measurements were performed in 90°-scattering geometry at temperatures between 6 and 250 K and in magnetic fields up to 6 T by placing the sample in the cold bore of a split-coil magnet. Light emission was excited by either a Ti:sapphire laser (750 nm) or a He–Ne laser (633 nm) incident on the (001) growth surface. Light emitted from one of the cleavage mirrors with linear polarization either parallel (∥) or perpendicular (⊥) to the ML plane (see inset to Fig. 1) was analyzed by a triple(double)-grating

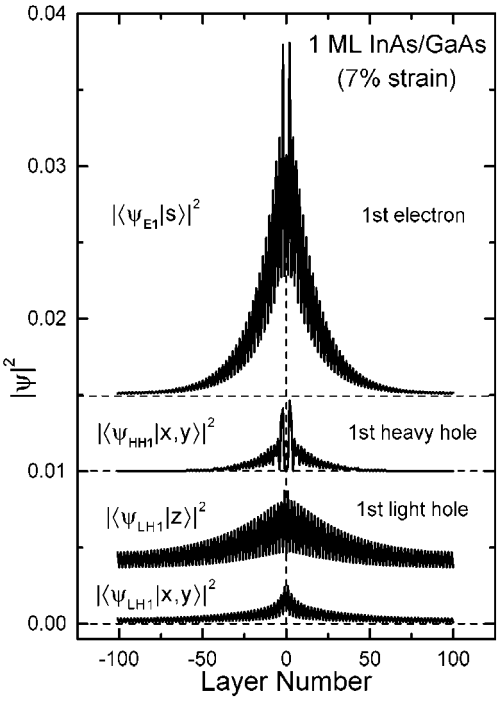

Fig. 2. Square modulus of the main atomic-orbital components of the wave functions for Γ point conduction and valence-band states bound to the InAs monolayer, as obtained from tight-binding calculations.

spectrometer and detected with a charge-coupled-device camera (photomultiplier).

Fig. 1 shows representative PL spectra of the InAs/GaAs ML sample measured in 90° geometry for two linear polarizations at different temperatures. For each polarization the PL emission is dominated by a single intense line, which is redshifted by 100 and 95 meV, respectively, from the energy of free excitons in bulk GaAs. The peak in ∥ polarization coincides with the only one apparent in spectra recorded in backscattering from the growth direction. A striking result concerns the change of the energy separation between both PL peaks from 4 meV at low temperature to 12 meV at 150 K.

For an assignment of the observed PL features we have calculated the electronic band structure by means of an sp^3s^* tight-binding (TB) model [26,27]. Details of the calculations are given elsewhere [19]. For our purpose we only consider the interaction between nearest neighbors but we include the effects of the large built-in biaxial stress due to the lattice mismatch and the spin–orbit coupling because relativistic corrections are important to obtain the proper orbital character of the valence-band states. In order to account for the band offsets, atomic-orbital energies for the InAs layers were shifted up by 250 meV [28]. Stress is introduced in the diagonal terms of the Hamiltonian such that the contribution arising from the tetragonal deformation affects

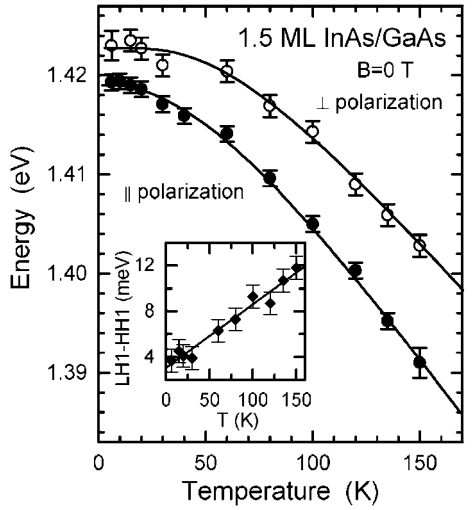

Fig. 3. Temperature dependence of the energy of the PL peak maxima for the two different linear polarizations. Solid lines represent the results of least-squares fits to the data using Eq. (1).

only the hole states. In contrast, the hydrostatic part has been taken into account by re-scaling the TB interaction parameters through the $d^{-\eta_{ll'}}$ rule, where d is the interatomic distance and $\eta_{ll'}$ is an exponent that depends on the pair of orbitals being considered [19].

For near band-gap states at the Γ point of the Brillouin zone the TB calculations predict the existence of a single electron (E1) state but two hole levels close in energy (~15 meV), a heavy (HH1) and a light-hole (LH1) one, which are bound to the InAs monolayer. Their envelope wave function peaks at the InAs decaying exponentially into the GaAs barrier, as schematically shown in Fig. 2, where the square moduli of the main atomic-orbital components of the three bound states have been plotted in real space. As expected, the electron state has markedly s character, whereas the hole levels are p-like. The classification of hole states into *heavy* and *light* proceeds according to the corresponding angular momentum components of the envelope functions.[1] An important result concerns the much larger penetration depth of the LH1 wave function into the GaAs, as compared to the envelopes of the HH1 and E1 levels.

Based on the TB results we assign the lowest energy PL peak observed in spectra with parallel polarization to optical transitions from the bound electron state E1 to the hole ground state HH1, whereas the main PL line with perpendicular polarization corresponds to the recombination of light-hole excitons. In this way, we can also explain the clear polarization selection rules of the PL emission from the InAs ML. As indicated by the atomic-orbital decomposition, only the 1LH state picks up a p_z contribution giving rise to light emission with predominantly z polarization, i.e. perpendicular to the plane of the InAs layer. In contrast, the optical recombination between the s-like electron state and the 1HH level having only $p_{x,y}$ character is entirely polarized in the monolayer plane.

In Fig. 3 we plotted the energy position of the main PL peak in each polarization as a function of temperature. The solid curves through the data points represent the results of least-squares fits using two identical expressions given by Eq. (1); one to account for the thermal expansion and one for describing the effect of the electron–phonon interaction. The gap change due to thermal expansion was calculated according to [4]

$$\frac{\partial E_g}{\partial T} = -3\alpha B_0 \frac{\partial E_g}{\partial P}, \tag{2}$$

where α is the expansion coefficient, B_0 the bulk modulus and $\partial E_g/\partial P$ is the linear pressure coefficient of the band gap. Using literature data for GaAs [29,30], the curve given by Eq. (2) can be approximated very well by a Viña-like expression with $\alpha_{th} = 40(1)$ meV and $\beta_{th} = 221(3)$ K. The resulting gap renormalization parameters are $\alpha_{ph} = 7(2)$ and 9(4) meV and $\beta_{ph} = 55(15)$ and 110(30) K for the E1–HH1 and the E1–LH1 transition, respectively. The data of Fig. 3 show that the energy splitting between the 1HH and 1LH hole bound states increases strongly with temperature (at 150 K the splitting is three times larger than at 6 K). This behavior translates into a ~5 meV (55 K) larger β_{ph} coefficient and a slightly higher gap renormalization constant α_{ph} for the temperature dependence of the E1–LH1 transition as compared to the E1–HH1 one.

The temperature enhancement of the heavy–light hole splitting is a consequence of the different renormalization of hole energies by electron–phonon coupling. The heavy holes being strongly localized to the InAs plane couple via deformation-potential interaction with the confined phonon modes of the monolayer. In contrast, light holes extend more into the GaAs barrier, thus, picking up a large contribution from bulk vibrations. The optical modes in GaAs are on the average about 5 meV stiffer than the phonons associated with the InAs monolayer [25]. This explains the larger average phonon frequency β_{ph} needed to fit the temperature data for the E1–LH1 transition using Eq. (1).

Temperature-induced changes in the built-in biaxial strain can be ruled out as the origin of the observed effect. By considering the difference in the thermal expansion coefficient of InAs and GaAs [30] we find that the change in strain between 5 and 150 K is less than 1×10^{-4} being negligible against the 6.8% due to lattice mismatch. Nevertheless, the strongest experimental evidence in favor of the electron–phonon coupling, which, in addition, disqualifies entirely thermal strain as a cause of the hole-splitting enhancement, is obtained from magnetoluminescene.

The temperature dependence of the HH1–LH1 energy splitting is largely reduced by applying a strong magnetic field in the plane of the InAs ML. The results for the hole

[1] In Ref. [19], the light-hole states have been wrongly assigned due to the lack of the orbital decomposition at that time.

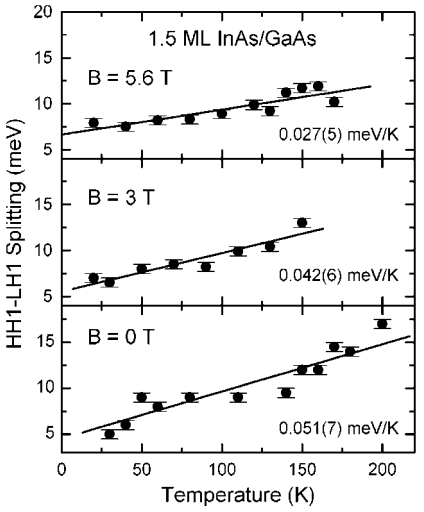

Fig. 4. Temperature dependence of the heavy–light hole energy splitting for three different magnetic fields. Solid lines represent linear fits to the data. The corresponding slopes are also indicated.

splitting as a function of temperature at three different fields between 0 and 6 T are shown in Fig. 4. The energy separation between bound heavy and light holes increases linearly with increasing temperature, the slope becoming smaller for large magnetic fields (at 5.6 T it is half of that without field). From Fig. 4 it is clear that the field affects the splitting mainly at low temperatures, i.e. the renormalization is principally due to zero-point vibrations. Thus, the coupling between the monolayer light holes and the GaAs phonons is reduced as a result of the increasing magnetic confinement in the growth direction, which is of the order of the magnetic length $l_0 = 25.7\ \text{nm}/\sqrt{B[T]}$. As the light holes penetrate less and less into the GaAs, the energy renormalization becomes weaker leading to a blueshift of the E1–LH1 optical transition energy at low temperatures. By these means we are able to effectively *tune* the dimensionality of the ML light holes, fact which shows up in the electron–phonon interaction. The magnetic field has no influence on the biaxial strain at all.

In conclusion, we have shown that in low-dimensional nanostructures the electron–phonon interaction can differ quantitatively for different states even though they might be very close in energy. This peculiar property finds its manifestation in the different temperature variation of energy levels stemming from the different overlap between wave function and phonon spectrum. Furthermore, we are able to influence the coupling between electronic and vibrational degrees of freedom by applying a strong magnetic field, which confines the carrier wave functions in the plane perpendicular to the field.

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