Localization of transverse optical phonons of GaAs in GaAs/Al$_x$Ga$_{1-x}$As periodic structures with paired quantum wells

A. G. Milekhin, Yu. A. Pusep, V. V. Preobrazhenskiĭ, B. R. Semyagin, and D. I. Lubyshev

Institute of Semiconductor Physics, Siberian Branch, Russian Academy of Sciences, 630090 Novosibirsk, Russia

(Submitted 9 March 1994)
Pis'ma Zh. Eksp. Teor. Fiz. **59**, No. 7, 471–474 (10 April 1994)

A localization of transverse optical phonons in GaAs layers separated by ultrathin Al$_x$Ga$_{1-x}$As barriers has been studied experimentally. It is shown that an AlAs layer 1 monolayer thick constitutes a barrier for GaAs phonons, while an Al$_x$Ga$_{1-x}$As layer with $x \leqslant 0.5$ is penetrable.

Progress in semiconductor technology has made it possible to fabricate periodic structures in which the layers have thicknesses comparable to interatomic distances. It thus becomes possible to study quantum size effects. In a description of the vibrational spectrum of periodic GaAs/AlAs structures with ultrathin layers, the localization of optical phonons must be taken into account. Since the dispersion of optical phonons of GaAs does not overlap that of optical phonons in AlAs, the phonons of each of these materials, which make up a periodic structure, are localized in the corresponding layers.

Some basic results on the localization of optical phonons have been found by a Raman-scattering method.[1] Because of the selection rules operating in Raman scattering for GaAs/Al$_x$Ga$_{1-x}$As superlattices grown in the (100) direction, only longitudinal optical (LO) vibrations can be observed. It was recently shown that IR spectroscopy can be used to study the localization of both longitudinal and transverse optical (TO) phonons. The selection rules for IR spectroscopy are such that only odd vibrational modes, with wave numbers

$$q_m=\frac{m\pi}{(n+\delta)a}, \tag{1}$$

can be observed. Here m is the index of the localized mode, n is the number of monolayers of the corresponding layer, and a is the thickness of a monolayer. The parameter δ is a measure of the depth to which a localized mode penetrates into the neighboring layers. As was shown in Ref. 3, for localized LO modes in GaAs/AlAs superlattices we have $\delta=1$. It has been found[4,5] experimentally that the LO phonons of GaAs are delocalized in GaAs/As$_x$Ga$_{1-x}$As superlattices if the barrier thickness is less than 20 Å ($x=0.4$) or 11 Å ($x=1$).

In the present letter we are reporting a study of localization of transverse optical phonons of GaAs in GaAs/Al$_x$Ga$_{1-x}$As periodic structures with paired quantum wells.

We studied the IR reflection spectra of $(GaAs)_n/(Al_xGa_{1-x}As)_t/(GaAs)_n/(AlAs)_m$ structures with paired quantum wells, where $m=10$, $n=3$, $t=1$ (this is the number of monolayers in the corresponding layer); and $x=1$, 0.5, 0.3 is the Al fraction in the $Al_xGa_{1-x}As$ solid solution (for samples 2, 3, and 4, respectively). The number of repetitions of these structures is 40. To determine the localization length of the quantized TO modes, we compared the IR spectra of structures with paired wells with spectra of $(GaAs)_k/(AlAs)_m$ superlattices with $k=3$ and 7 (samples 1 and 5, respectively) and $m=10$. In the case of a penetrable barrier, the localization lengths of quantized TO modes of GaAs of $(GaAs)_7/(AlAs)_{10}$ superlattices and of structures with paired quantum wells should be the same.

The samples were grown by molecular beam epitaxy on a Katun'-S apparatus on Si-doped GaAs substrates (AGNK-4s material, with $n_{Si}=2\times10^{18}$ cm^{-3}), oriented in the (100) direction. The doped substrates made it possible to eliminate interference in the substrate. The thicknesses of the layers of the superlattice were monitored by detecting oscillations in the intensity of the specular reflection in the pattern of reflection high-energy electron diffraction.

The IR reflection spectra were recorded on a Bruker IFS-113V IR Fourier spectrometer as the light was incident normally on the sample, at a temperature of 77 K. The resolution was 1 cm^{-1} over the entire spectral range. Spectra of the derivative of the reflection, $dR/d\omega$, were analyzed to determine the frequencies of the observed vibrational modes highly accurately.

Figure 1 shows derivatives of the experimental IR reflection spectra of the test samples in the frequency region of a TO phonon of GaAs. The structural features in the spectra of the derivative marked by the arrows here correspond to the TO_1 and TO_3 modes, localized in the GaAs layers. The knee in the spectra at frequencies below 260 cm^{-1} corresponds to a low-frequency plasmon–phonon mode in the substrate. The position of this knee depends on the doping level. As can be seen from curves 1 and 2 in Fig. 1, the frequencies of the localized TO modes of the $(GaAs)_3/(AlAs)_{10}$ and $(GaAs)_3/(AlAs)_1/(GaAs)_3/(AlAs)_{10}$ structures are the same. This agreement is evidence that the TO phonons of GaAs are localized in GaAs layers with a thickness of three monolayers. An AlAs layer one monolayer thick thus constitutes a barrier to the penetration of TO vibrations of the GaAs crystal lattice into neighboring quantum wells.

If the paired quantum wells are separated by a layer of an $Al_xGa_{1-x}As$ solid solution with $x\leqslant0.5$ and a thickness of one monolayer, the spectra of the derivative of the reflection of the $(GaAs)_3/(Al_xGa_{1-x}As)_1/(GaAs)_3/(AlAs)_{10}$ superlattice contain a high-frequency shift of the line of the GaAs TO_3 mode (curve 3 corresponds to $x=0.5$, and curve 4 to $x=0.3$). Such a shift may be due to an increase in the localization length of the corresponding vibrational modes, if the $Al_xGa_{1-x}As$ barrier is penetrable for the localized TO modes. In this case the TO phonons of GaAs are localized over the total thickness of the layer consisting of the two quantum wells separated by the ultrathin $Al_xGa_{1-x}As$ barrier. Essentially no changes in the TO_1 frequency are observed because of the weak dispersion of TO phonons of GaAs at small wave numbers.

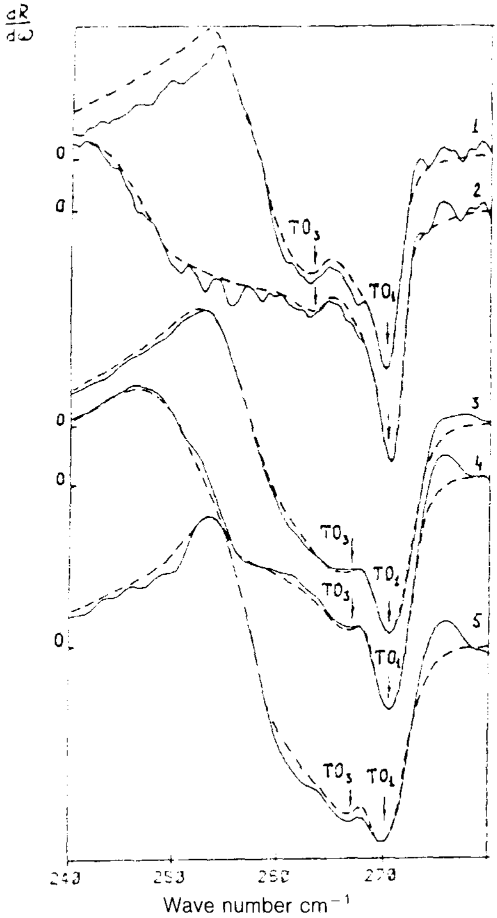

FIG. 1. Derivatives of the experimental (solid curves) and theoretical (dashed curves) IR reflection spectra of superlattices. *1*—A $(GaAs)_3/(AlAs)_{10}$ superlattice; *2*— $(GaAs)_3/(AlAs)_1/(GaAs)_3/(AlAs)_{10}$; *3*—$(GaAs)_3/(Al_{0.5}Ga_{0.5}As)_1/(GaAs)_3/(AlAs)_{10}$; *4*—$(GaAs)_3/(Al_{0.3}Ga_{0.7}As)_1/(GaAs)_3/(AlAs)_{10}$; *5*—$(GaAs)_7/(AlAs)_{10}$.

Confirmation that localized TO modes penetrate through a monolayer barrier of solid solution comes from the exact agreement of (on the one hand) the frequencies of the localized TO_i modes of GaAs in periodic $(GaAs)_3/(Al_xGa_{1-x}As)_1/(GaAs)_3/(AlAs)_{10}$ structures with $x=0.3$ and 0.5 with (on the other) the frequencies of TO_i modes localized in a $(GaAs)_7/(AlAs)_{10}$ lattice (curve 5 in Fig. 1) in a GaAs layer seven monolayers thick.

The exact frequencies of the localized modes were found by fitting the theoretical spectrum to the experimental one. Theoretical spectra were calculated by the $E-H$ matrix method for layered structures.[6] It was assumed that each layer is isotropic and can be described by a dielectric function

$$\epsilon_{1(2)}=\epsilon_{\infty 1(2)}+\sum_i \frac{\Omega^2_{pi1(2)}}{\omega^2_{ti1(2)}-\omega^2+i\omega\gamma_{i1(2)}}, \tag{2}$$

where $\epsilon_{\infty 1(2)}$ is the high-frequency dielectric function, and $\omega_{ti1(2)}$, $\Omega_{pi1(2)}$, and $\gamma_{i1(2)}$

TABLE I.

	Substrate		Parameters of GaAs layers					
Sample	Ω_p	γ_p	ω_{t1}	Ω_{p1}	γ_1	ω_{t3}	Ω_{p3}	γ_3
1	1380	55	270.5	370	2.5	264.2	260	5.1
2	1160	50	270.5	370	2.3	264.5	267	5.6
3	1400	55	270.5	373	2.8	267.1	269	5.6
4	1290	60	270.5	370	2.8	267.1	269	5.2
5	1400	49	270.3	373	2.8	267.1	350	4.2

Note. All values are expressed in units of cm^{-1}.

are the frequency of the *i*th localized TO mode and the plasma frequency and attenuation coefficient of the *i*th mode. The subscript 1 corresponds to the GaAs layer, and 2 to the AlAs layer. The summation is over all odd modes, since even modes do not have a dipole moment and do not contribute to the dielectric function.

The dashed curves in Fig. 1 are the theoretical spectra which agree best with experiment. The parameters emerging from the fitting procedure are listed in Table I.

In summary, we have studied the vibrational spectrum of $(\text{GaAs})_3/(\text{Al}_x\text{Ga}_{1-x}\text{As})_1/(\text{GaAs})_3/(\text{AlAs})_{10}$ structures with paired quantum wells in the frequency region of the TO phonon of GaAs. It has been shown that a barrier one monolayer thick with $x=1$ results in a localization of GaAs TO phonons in the paired GaAs quantum wells, while a barrier with an Al content $x \leqslant 0.5$ is penetrable.

[1] M. Cardona, *Light Scattering in Solids V* (Springer-Verlag, Heidelberg, 1989).

[2] Yu. Pusep *et al.*, Superlattices and Microstructures **13**, 115 (1993).

[3] B. Jusserand and D. Paquet, Phys. Rev. Lett. **56**, 1752 (1986).

[4] D.-S. Kim *et al.*, Phys. Rev. Lett. **68**, 1002 (1992).

[5] A. Ishibashi *et al.*, Phys. Rev. B **33**, 2887 (1986).

[6] B. Heinz, *Optische Konstanten von Halbleiter-Mehrschicht-Systemen*, Doctoral Dissertation (R.-W.T.H., Aachen, 1991).

Translated by D. Parsons