Trapped phonons in the reflection spectra of GaAs/AlGaAs superlattices

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Structural features attributable to the trapping of transverse optical phonons in the layers of GaAs/AlGaAs superlattices have been observed in reflection spectra. The dispersion of TO phonons in AlAs has been measured for the first time.

Localization (confinement) of optical phonons resulting from their space quantization in the layers of GaAs/AlGaAs superlattices (SL) was detected in experimental studies of the Raman scattering of light.[1,2] In superlattices whose axis is parallel to one of the major axes of a cubic crystal the selection rules allow Raman scattering only by the longitudinal optical phonons, while both longitudinal and transverse optical lattice vibrations are active in the IR spectra.

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In this letter we present for the first time the reflection spectra of GaAs/AlGaAs superlattices, which show that the optical phonons are trapped.

We studied the superlattices which were grown by the molecular-ray epitaxy method at the Max Planck Institute of Solid State Research (FRG) and at the Institute of Semiconductor Physics, Academy of Sciences of the USSR, on GaAs substrates oriented in the [100] direction. The reflection spectra were recorded using a Bruker IFS-113V Fourier spectrometer and a helium-cooled germanium bolometer was used as a photodetector. The reflection was measured at an angle close to the normal angle ($\theta \simeq 10^\circ$). The spectral resolution was 0.3 cm^{-1} over the entire range of measured frequencies.

The superlattices which we studied are characterized by the absence of overlapping of the dispersion relations of the optical phonons in the adjacent layers. Under these conditions, the phonons are trapped in the SL layers, while their spectrum becomes a discrete spectrum, in which the wave numbers which are multiples of π/d are resolved; here d is the thickness of the corresponding layer.

Figure 1 is a spectral dependence of the reflection of $(\mathrm{GaAs})_{10}(\mathrm{AlAs})_{10}$ and $(\mathrm{GaAs})_{17}(\mathrm{AlGaAs})_{17}$ superlattices, recorded in the region of transverse optical vibrations in the GaAs layers. Here the numerals specify the number of monatomic layers of the corresponding layer of superlattices. The inset in Fig. 1 shows the total reflection spectrum of a GaAs/AlAs superlattice which contains the bands of the residual rays of the GaAs and AlAs layers. The reflection steps indicated by the arrows are attributable to the localized TO modes. Figure 2 shows the spectra of the reflection

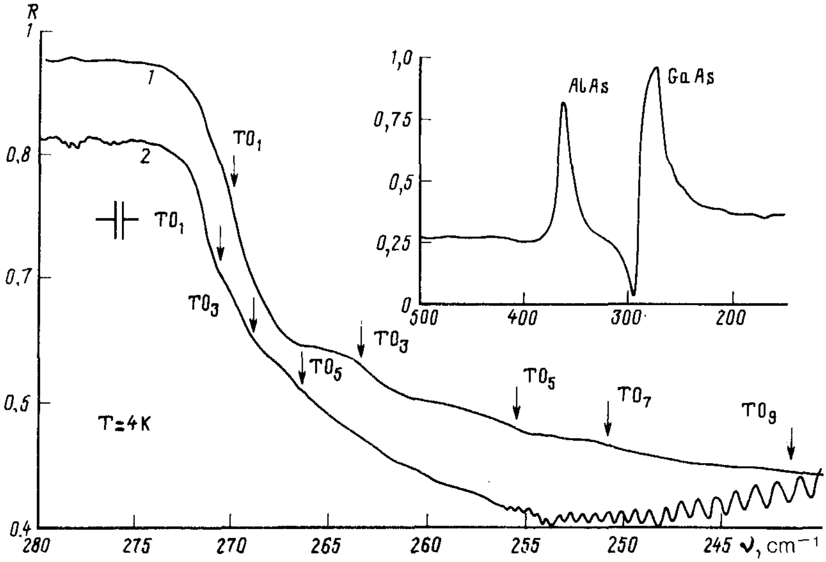

FIG. 1. Reflection spectrum 1—$(\mathrm{GaAs})_{10}(\mathrm{AlAs})_{10}$ superlattice (100×); reflection spectrum 2—$(\mathrm{GaAs})_{17}(\mathrm{Al}_{0.35}\mathrm{Ga}_{0.65}\mathrm{As})_{17}$ (30×), measured in the region of transverse optical oscillations at $T = 4.2$ K.

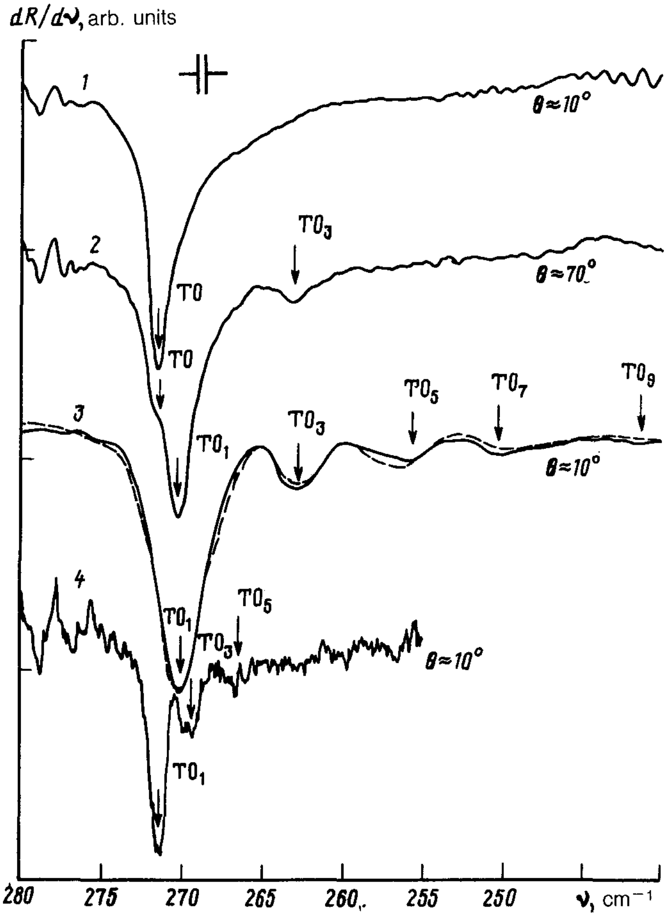

FIG. 2. Spectra of the reflection derivative. 1—GaAs single-crystal film ($d \simeq 1.7$ μm); 2—$(GaAs)_{10}(AlAs)_{10}$ superlattice with $\theta \simeq 70°$; 3—$(GaAs)_{10}(AlAs)_{10}$ superlattice with $\theta \simeq 10°$; 4—$(GaAs)_{17}(Al_{0.35}Ga_{0.65}As)_{17}$ superlattice with $\theta \simeq 10°$. Dashed line—Calculation.

derivative $\partial R / \partial v$, whose structural features make it possible to determine very accurately the frequencies of the trapped modes that have been observed. Curve 1 corresponds to the reflection spectrum of a GaAs film ($d \approx 1.7$ μm), whose minimum is due to the transverse optical vibrations (at 271.6 cm^{-1}). In the spectra of the reflection derivative of the superlattices recorded at an angle close to the normal angle (curves 3 and 4), we see clearly the defined minima which correspond to the trapped modes.

It is clear that an increase in the angle of incidence leads to a decrease of the phonon momentum component, which is directed along the axis of the superlattice, and to an increase of the momentum component in the perpendicular direction. Since the motion of phonons along the layers of the superlattice is not quantized in the reflection spectra recorded at a large angle of incidence of light, the structural feature caused by the bulk *TO* phonon should be observed. This circumstance is illustrated by curve 2 in Fig. 2, which is the derivative of the reflection spectrum of the superlattice recorded at an angle of $\theta \approx 70°$; here the intensity of the localized modes decreases and a minimum corresponding to a bulk *TO* phonon appears.

To determine the spectral dependence of the reflection of the superlattice, we must calculate its dielectric constant which is given by the following expression in the case of a normal incidence of light:[3]

$$\epsilon_{SL}(\omega) = \frac{1}{d_1 + d_2}(\epsilon_1 d_1 + \epsilon_2 d_2), \tag{1}$$

where d_1 and d_2 are the thicknesses of layers of the superlattices, and ϵ_1 and ϵ_2 are the dielectric constants of the corresponding layers.

Following Ref. 4, the optical phonon localization in the SL layers can be determined from the dielectric constant of the multimode crystal; for n modes, which are active in the RI spectra, we then have:

$$\epsilon_{1,2}(\omega) = \epsilon_\infty \left[1 + \sum_j^n \frac{A_j(\omega_{Loj}^2 - \omega_{Toj}^2)}{\omega_{Toj}^2 - \omega^2 + i\omega\Gamma_j}\right], \tag{2}$$

where ϵ_∞ is the rf dielectric constant of the layer, and j, ω_{Loj} and ω_{Toj} are the order of the mode and the optical frequencies corresponding to this mode. The coefficients A_j characterize the interaction of the mode with the light, which determines its dipole moment:

$$P_j = \frac{(e^*)^2 E}{M(\omega_{Toj}^2 - \omega^2)} A_j = \frac{(e^*)^2 E \cdot C}{M(\omega_{Toj}^2 - \omega^2)m} \sum_i^m \sin\left(\frac{2\pi z_i}{\lambda_{Toj}}\right), \tag{3}$$

where the sum is taken over all m atoms in the SL layer, e^* and M are the effective charge and the reduced unit cell mass, E is the electric field strength, ω_{Toj} and λ_{Toj} are the frequency and wavelength of the jth mode, $z_i = (d/m)i$ is the coordinate of the ith atom in the layer (z runs parallel to the axis of the SL) and C is an adjustable parameter which is determined by means of the sum rule:[4]

$$C \sum_j \left(\frac{\omega_{Loj}^2}{\omega_{Toj}^2} - 1\right) A_j = \frac{\epsilon_0}{\epsilon_\infty} - 1. \tag{4}$$

TABLE I.

j	1	3	5	7	9
A_j	0,566	0.175	0.089	0,046	0.014
ν_{Loj}, cm^{-1}	294	291	286	280	272
ν_{Toj}, cm^{-1}	271	265	260	253	244
Γ_j, cm^{-1}	3.3	6.5	7.0	8.0	8.0

Only the coefficients for the localized odd modes are nonvanishing, as follows from (3).

Using relations (1) and (2), we calculated the reflection spectra of the SL under study; the longitudinal frequencies ω_{Loj} in (2) in this case were determined from the dispersion of the LO phonons[2] with a wave number $k_j = (\pi/d)j$ corresponding to each localized mode.

The spectrum of the reflection derivative calculated for the GaAs layer of the GaAs/AlAs superlattice, whose thickness amounts to ten monolayers, is shown by the dashed line in Fig. 2. A good agreement between the experiment and calculation was obtained when the following parameters were used: $\epsilon_\infty = 11$, $\epsilon_0 = 12.8$, and $C = 0.89$; the remaining calculated parameter values are listed in Table I.

The dispersion of transverse optical phonons in GaAs and AlAs, determined from the reflection spectra, is shown in Fig. 3. The dispersion relation of TO phonons in

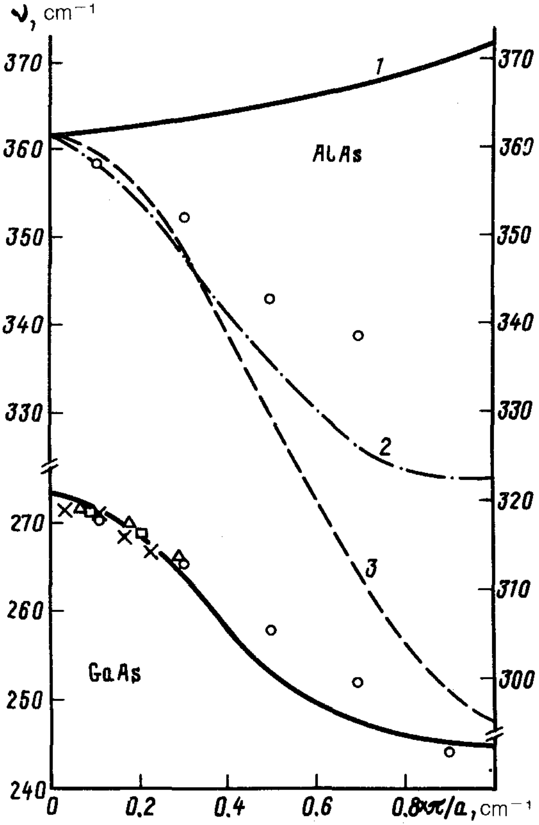

FIG. 3. Dispersion of transverse optical phonons in GaAs and AlAs. The wave numbers are given in π/a, where a is the lattice constant. The symbols on the dispersion curve for GaAs correspond to the position of the trapped TO modes in the spectrum for GaAs layers of various thicknesses. ○—Ten monolayers; □—14 monolayers; △—17 monolayers; ×—30 monolayers.

GaAs, determined from the reflection spectra, is in just as good agreement with the theory[5] as the data obtained in the study of the forbidden Raman scattering.[2] There are no experimental data on the dispersion of optical phonons for AlAs. Theoretical calculations[6,7] predict various dependences of the *TO* phonon frequencies on the wave number in AlAs (curves 1 and 3 in Fig. 3). Curve 1 was calculated with allowance for the covalent nature of the interatomic bonds and curve 3 was calculated with allowance for the covalent and metallic bonds. A qualitative agreement with curve 3 confirms the assumption that both types of bonds are important in the III–V compounds.[8] The dependence calculated by scaling the dispersion of *TO* phonons in GaAs is in relatively good agreement with the experimental data (curve 2).

We note, in conclusion, that the localized *TO* modes were observed in both layers of GaAs/AlAs superlattices, but were not observed in the solid solution layers of GaAs/AlGaAs superlattices. This circumstance seems to be attributable to the shorter mean free path of phonons in the solid solution.

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