Penetration of optical vibrations localized in the layers of GaAs/AlAs periodic structures into the barrier according to reflection spectra

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Reflection spectra have been used for a study of optical vibrational modes localized in the GaAs layers of periodic $(GaAs)_n(AlAs)_m$ structures. Spectras indicating a partial penetration of GaAs phonons into the neighboring AlAs layers are presented. The penetration depth is calculated in the model of a linear chain.

A study of the energy spectrum of phonons localized in thin layers can reveal information about the dispersion of the vibrational spectrum of crystals of interest. Because of the difference between the frequencies of the optical phonons of GaAs and AlAs, the optical vibrations in periodic $(GaAs)_n(AlAs)_m$ structures (n and m are the numbers of GaAs and AlAs monolayers, respectively) localize in both layers. The AlAs layers serve as barriers for the GaAs phonons, and vice versa. We have previously observed[1] structural features in reflection spectra which stemmed from the direct interaction of the light with vibrational modes localized in the layers of $(GaAs)_n(AlAs)_m$ superlattices. In this case, in contrast with Raman scattering, the interaction of the light with the phonons is a first-order process. As a result, interpreting the experimental results becomes a much simpler matter.

A problem which arises in attempts to describe the vibrational properties of periodic structures is the effect of the interfaces between the layers. For phonon modes which are localized in layers, this problem becomes one of determining the depth to which the given mode penetrates into the neighboring layer. As has been shown in several theoretical studies (e.g., Refs. 2 and 3), the penetration depth for

$(GaAs)_n(AlAs)_m$ periodic structures is on the order of the distance between atomic planes. A penetration of localized vibrations into neighboring layers has been observed in a study of the Raman effect in superlattices with ultrathin layers, with thicknesses from 1 to 6 monolayers.[4]

In this letter we are reporting reflection spectra of the optical vibrational modes localized in the GaAs layers of periodic $(GaAs)_n(AlAs)_m$ structures. These spectra indicate a partial penetration of these modes into the neighboring AlAs layers.

We studied periodic $(GaAs)_n(AlAs)_m$ structures grown by molecular beam epitaxy on GaAs substrates oriented along the [001] direction, with 50 repetitions. The reflection spectra were recorded in the region of transverse optical vibrations of GaAs at liquid-helium temperature with the help of a Bruker IFS-113V Fourier spectrometer. A liquid-helium-cooled germanium bolometer was used as photodetector. The reflection was measured at an angle near the normal. As was shown in Ref. 1, minima of the reflection derivative $dR/d\nu$ correspond to the frequencies of localized *TO* phonons. The size of these minima decreases monotonically with increasing mode index. This decrease in size stems from a decrease in the part of the dipole moment that has not been canceled. The penetration of localized phonons into the barrier gives rise to an increment, which increases the dipole moment of the localized mode. The dipole moment of the higher-index modes should evidently change to a greater extent. In the

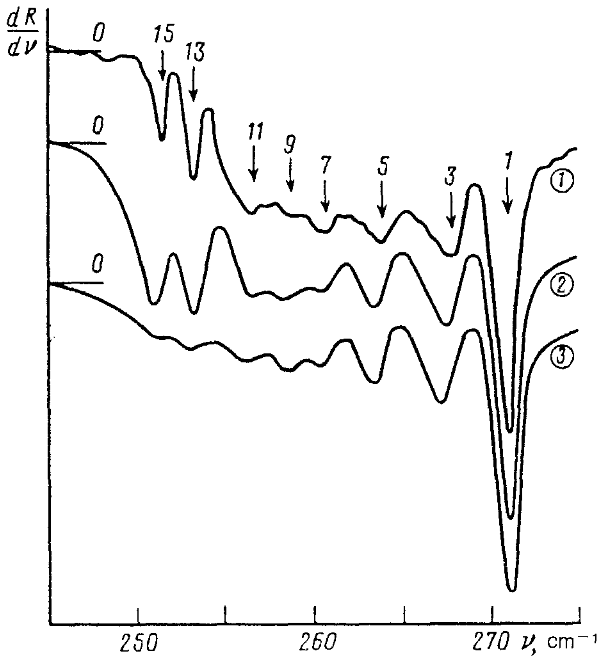

FIG. 1. Spectra of the derivative $dR/d\nu$ of a $(GaAs)_{17}(AlAs)_{17}$ periodic structure. 1—Experimental results for $T = 4.2$ K; 2—a calculation from (2) with the parameters of the localized modes given in Table I; 3—results calculated with the coefficients A_j determined in the absence of penetration ($\delta = 0$), with otherwise the same parameter values as were used in the calculation of spectrum 2.

structures studied by us, we observed an increase in the size of the dR/dv minima corresponding to *TO* vibrational modes localized in the GaAs layers. This increase stemmed from a change in the dipole moment of these modes, itself a consequence of penetration into the barrier.

Figure 1 shows a spectrum of the derivative of the reflection of a periodic $(GaAs)_{17}(AlAs)_{17}$ structure. The amplitudes of the first five localized *TO* modes fall off monotonically with increasing mode index, while the intensity of the last modes increases. The reflection spectrum of the periodic structure in the phonon-excitation region can be calculated with the help of the dielectric function

$$\epsilon_{sl}(\omega) = (\epsilon_1 d_1 - \epsilon_2 d_2)/(d_1 - d_2), \qquad (1)$$

where d_1, d_2 are the layer thicknesses, and ϵ_1, ϵ_2 are the dielectric functions of the corresponding layers. The localization of the phonons which are propagating in the direction perpendicular to the layers gives rise to standing waves, whose period is determined by the thickness of the layer, and whose frequency is determined by the

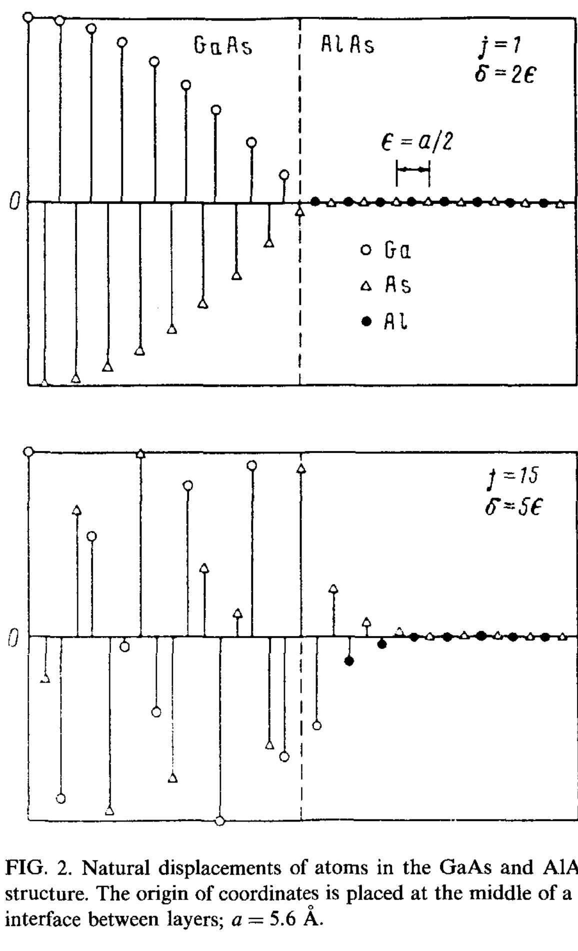

FIG. 2. Natural displacements of atoms in the GaAs and AlAs layers of a $(GaAs)_{17}(AlAs)_{17}$ periodic structure. The origin of coordinates is placed at the middle of a GaAs layer. The dashed line represents an interface between layers; $a = 5.6$ Å.

TABLE I. Parameters of localized vibrations of a $(GaAs)_{17}(AlAs)_{17}$ periodic structure.

j	1	3	5	7	9	11	13	15
ω_{Lj}	294	292	287	282	277	272	262	262
ω_{Tj}	271	268	264	261	259	256,6	253,8	251,5
γ_j	1,7	3	3	3	3	3	2,5	2,5
A_j	0,449	0,153	0,090	0,063	0,045	0,036	0,089	0,073
δ_j	2	2	2	2	2	3	5	6
$A_j(\delta=0)$	0,49	0,16	0,097	0,068	0,052	0,041	0,033	0,027

The frequencies ω and the damping parameters γ are expressed in units of reciprocal centimeters, while δ is expressed in units of monolayers (ϵ).

phonon dispersion in the bulk crystal. The dielectric function of a layer in which there is a localization of phonons is determined by the sum of the contributions from each localized mode in accordance with

$$\epsilon_{1,2}(\omega) = \epsilon_{\infty 1,2}[1 + \sum_j A_j(\omega_{Lj}^2 - \omega_{Tj}^2)/(\omega_{Tj}^2 - \omega^2 - i\omega\gamma_j)], \quad (2)$$

where $\epsilon_{\infty 1,2}$ are the high-frequency dielectric constants of the corresponding layers, ω_{Lj} and ω_{Tj} are the frequencies of longitudinal and transverse optical vibrations characterizing the jth localized mode, γ_j is the damping of this mode, and A_j are oscillator strengths. These strengths characterize the interaction of the mode with the light and are determined by the dipole moment of the mode.

We adopted the model of a linear chain for an approximate calculation of the oscillator strengths of the localized *TO* modes.[5] Figure 2 shows the natural displacements of the atoms in the layers of the $(GaAs)_{17}(AlAs)_{17}$ structure for the first and fifteenth modes. Curve 2 in Fig. 1 shows the reflection derivative spectrum calculated with the help of the calculated oscillator strengths for the localized modes. The parameters of the localized modes which lead to the best agreement between theory and experiment are listed in Table I. It can be seen from this table that the penetration depth $\delta = 2\pi/\mathrm{Im}\, q$ increases for the latter localized modes ($\mathrm{Im}\, q$ is the imaginary part of the wave number, a measure of the damping of the mode in the barrier). This result is a consequence of the approximate equality of the frequencies of acoustic vibrations of AlAs, on the one hand, and the frequencies of optical vibrations of GaAs, on the other, in the wave-number region near the edge of the Brillouin zone. The values given for the penetration depth in Table I correspond well to the values of the $\mathrm{Im}\, q$ calculated by Colvard *et al.*[2] for GaAs phonons in the AlAs layers of $(GaAs)_n(AlAs)_m$ superlattices. Also given in Table I are oscillator strengths of localized modes as calculated in the absence of penetration ($\delta = 0$). The reflection derivative spectrum for this case shows a monotonic decrease in the size of the minima corresponding to the localized modes (curve 3 in Fig. 1).

It can be concluded from the results of this study that the optical vibrations localized in the GaAs layers of periodic $(GaAs)_n(AlAs)_m$ structures penetrate partially into the neighboring AlAs layers. The penetration depth increases for modes with wave numbers close to the Brillouin edge.

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