

Raman scattering in stressed CdTe/Zn_xCd_{1-x}Te superlattices

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The Raman scattering spectra of stressed CdTe/Zn_xCd_{1-x}Te superlattices have been studied. The distribution of strain among layers has been established unambiguously for the first time.

Stressed CdTe/Zn_xCd_{1-x}Te superlattices are attracting much interest because they hold promise for practical applications. The characteristics of the potential barriers at the interface can be controlled and varied over a wide range because of the significant difference (up to 6.5%) in the lattice constants and because of the large strain energies. The slight disruption of the valence bands makes it possible to produce superlattices of both the first and second types, by varying the magnitude and sign of the deformation. There is the further possibility of the rather exotic situation in which the superlattice is at once a superlattice of the first type for heavy holes and a superlattice of the second type for light holes.

The band structure of the CdTe/Zn_xCd_{1-x}Te superlattices is thus determined to a large extent by the distribution of strain among layers. The data on this point, however, are contradictory.^{1,2} Jackson *et al.*² have asserted, on the basis of a study of Raman scattering, that there exists a “free-standing” configuration in which the lattice constant in the plane perpendicular to the axis of the superlattice depends on only the ratio of layer thicknesses:

$$a_{\parallel} = [(a_{\text{CdTe}} + a_{\text{ZnCdTe}})d_{\text{ZnCdTe}}/d_{\text{CdTe}}][1 + (d_{\text{ZnCdTe}}/d_{\text{CdTe}})]^{-1}. \quad (1)$$

On the other hand, Menendez *et al.*¹ have shown that the strain distribution does not always correspond to a free-standing configuration. The situation here is substantially different from that in the conventional III–V superlattices,³ in which a free-standing configuration is observed when the number of periods is large. It has been shown in several places^{1,2,4} that CdTe/ZnCaTe superlattices can be free-standing configurations even if the number of periods is small. The problem we took up in the present study was to determine the behavior of the CdTe/Cd_{1-x}Zn_xTe superlattice.

The structural quality of stressed superlattice depends strongly on the thickness of the constituent layers. If the thickness of these layers is greater than a critical d_c , the stress relaxes through the formation of mismatch dislocations. Since the studies reported in Refs. 1 and 2 were carried out on CdTe/ZnTe superlattices with layer

thicknesses greater than $d_c = 6$ monolayers (ML) for this heterostructure,⁵ the results found there depended on the extent of the relaxation and on its mechanism. We believe that this situation is responsible for the discrepancies between the results of Refs. 1 and 2. In order to obtain reliable data on the strain distribution in these superlattices and thus on the band structure of these superlattices, it is necessary to carry out measurements on a fairly large number of samples, with thicknesses below the critical value. Such a study becomes possible when $\text{Zn}_x\text{Cd}_{1-x}\text{Te}$ is used as the material for the barrier layers; the critical thickness for such layers is considerably larger [$d_c > 50$ monolayers (ML) for $x = 0.2$].

We studied $\text{CdTe}/\text{Zn}_x\text{Cd}_{1-x}\text{Te}$ superlattices grown by molecular epitaxy. The substrate was semi-insulating GaAs, on which a thick ($\approx 1\text{-}\mu\text{m}$) buffer layer of CdTe was deposited. The layer growth was monitored *in situ* on the basis of the oscillations in the intensity of the specular peak in high-energy electron diffraction. We were thus able to measure the layer thicknesses directly. Raman spectra were recorded at 77 K and 300 K in the Brewster quasi-backscattering geometry during excitation by an argon laser with $\lambda = 514.5$ nm.

Figure 1 shows Raman spectra of five samples, for which the thickness of the $\text{Zn}_{0.2}\text{Cd}_{0.8}\text{Te}$ layers was the same, while the thicknesses of the CdTe layers were different. In these spectra we clearly see a line 1, which shifts from 158 cm^{-1} to 167.5 cm^{-1} as the thickness of the CdTe layers increases, and a line 2, which remains at the same position (178 cm^{-1}) in all the spectra. Line 1 intensifies in proportion to the increase in the thickness of the CdTe layers in the superlattice. The frequency of this line in the superlattice with the thickest layers is the same as the frequency of an *LO* phonon in unstressed bulk CdTe. As the thickness of the CdTe layers is reduced, a shift of this line in the low-energy direction is caused by a localization of phonons⁶ in the CdTe layers, according to our calculations (Fig. 2). On the basis of these results we concluded that line 1 is due to Raman scattering by *LO* phonons in the CdTe layers and that these layers are not stressed in the superlattice. It is reasonable to suggest that the second line observed in the spectra arises from *LO* phonons in the $\text{Zn}_x\text{Cd}_{1-x}\text{Te}$ layers. We should point out that the width of each of these lines is approximately equal to the width of the phonon lines in bulk samples. This approximate agreement suggests a high crystal quality of the layers. It also suggests that a stress relaxation does not occur. In this case the $\text{Zn}_x\text{Cd}_{1-x}\text{Te}$ layers in the superlattice should be stressed, and their lattice constant in the plane of the superlattice should be the same as that of the CdTe layers, i.e., equal to the bulk value in CdTe. Stress shifts the frequencies of the *LO* phonons of the $\text{Zn}_x\text{Cd}_{1-x}\text{Te}$ barrier layer by an amount $\Delta\omega_{LO} = (\delta\omega/\delta p) \cdot X$, where $\delta\omega/\delta p$ is the baric coefficient of the shift of the phonon frequency, and X is a component of the stress tensor in the plane of the layers. For a superlattice with the (100) orientation we would have

$$X = \frac{\alpha_{\text{CdTe}} - \alpha_{\text{ZnCdTe}}}{\alpha_{\text{ZnCdTe}}} \cdot \frac{1}{(S_{11} + S_{12})_{\text{ZnCdTe}}}, \quad (2)$$

and this quantity would depend on only the Zn concentration. Substituting in some numerical values,^{7,8} we find $\Delta\omega_{LO} = 2.8\text{ cm}^{-1}$. The frequency of an *LO*₁ phonon in unstressed $\text{Zn}_{0.2}\text{Cd}_{0.8}\text{Te}$ is⁷ 183 cm^{-1} . In view of the strain-related shifts calculated

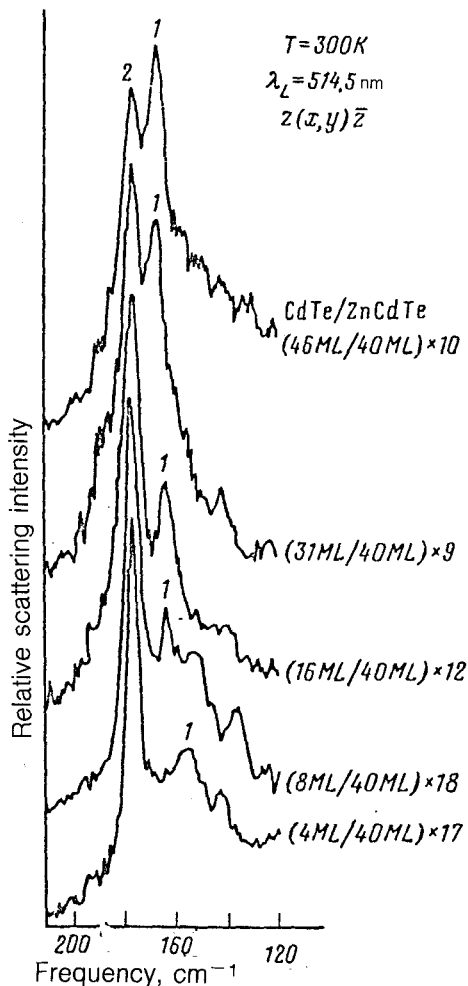


FIG. 1. Raman spectra of $\text{Zn}_{0.2}\text{Cd}_{0.8}\text{Te}/\text{CdTe}$ superlattices with various thicknesses of the CdTe layers.

above, we conclude that we should observe a line at the frequency $\Delta\omega_{LO_1} = 180.2 \text{ cm}^{-1}$ in the Raman spectra of superlattices with a $\text{Zn}_{0.2}\text{Cd}_{0.8}\text{Te}$ barrier layer (Fig. 1). The value found for ω_{LO_1} is slightly higher than the frequency of line 2, but the discrepancies here may have occurred because we were obliged to use approximate values for the elastic constants and the baric coefficient for the shift of the resonant frequencies for $\text{Zn}_x\text{Cd}_{1-x}\text{Te}$. We found similar results for all the $\text{Zn}_{0.2}\text{Cd}_{0.8}\text{Te}/\text{CdTe}$ superlattices which we studied, with the various thicknesses of the $\text{Zn}_{0.2}\text{Cd}_{0.8}\text{Te}$ and CdTe layers. In addition, we measured the Raman spectra of a $\text{Zn}_{0.1}\text{Cd}_{0.9}\text{Te}(10 \text{ ML})/\text{CdTe}(10 \text{ ML})$ superlattice, in which the difference between lattice constants was smaller, so the shifts of the phonon frequencies should be smaller. As in the case of the $\text{Zn}_{0.2}\text{Cd}_{0.8}\text{Te}/\text{CdTe}$ superlattice, the position of the CdTe LO-phonon peak is the same as that of the bulk peak, and we detected a line at a frequency of 175 cm^{-1} .

The frequency of this line corresponds fairly well to the value of 175.5 cm^{-1} calculated for an LO_1 phonon in $\text{Zn}_{0.1}\text{Cd}_{0.9}\text{Te}$ "stretched out" to the lattice constant of CdTe.

These results show unambiguously that the strain distribution in these superlattices with layer thicknesses smaller than the critical thickness is determined by the lattice constant of the buffer layer. In other words, there is a coherent growth, in the course of which the superlattice has a pseudomorphic structure, and the lattice constant of the buffer material is reproduced from layer to layer. On the other hand, the results found here cannot be explained on the basis of a free-standing configuration, since in this case there should also be shifts of the phonon lines in CdTe. According to (1), the value of these shifts would be determined by the ratio of the layer thicknesses in Fig. 2.

This strain distribution is observed over the entire Zn concentration range studied. Figure 3 shows the Raman scattering spectrum of a $\text{ZnTe}(2 \text{ ML})/\text{CdTe}(10 \text{ ML})$

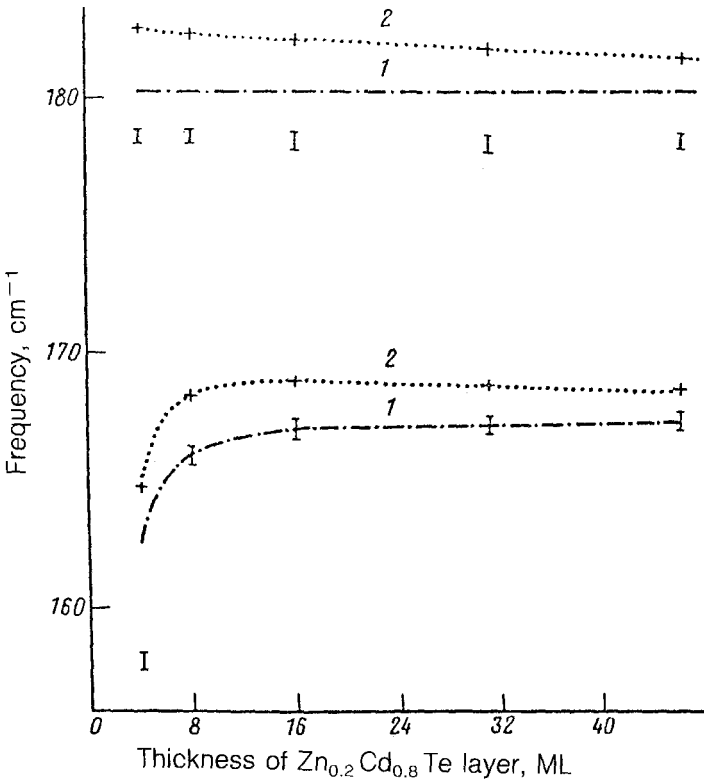


FIG. 2. Frequencies of the Raman-scattering lines of $\text{Zn}_{0.2}\text{Cd}_{0.8}\text{Te}/\text{CdTe}$ superlattices versus the thickness of the $\text{Zn}_{0.2}\text{Cd}_{0.8}\text{Te}$ layer. 1—Frequencies calculated for a coherent stress configuration; 2—frequencies calculated for a free-standing configuration. The shift of the phonon frequencies associated with the localization of phonons in the layers was incorporated in the calculations.

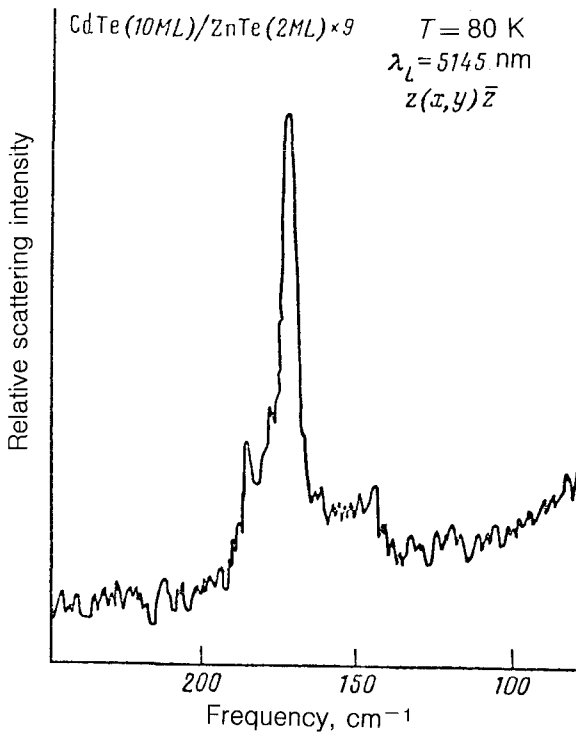


FIG. 3. Raman scattering spectrum of a ZnTe/CdTe superlattice.

superlattice on a CdTe buffer layer at $T = 77 \text{ K}$. The 172-cm^{-1} line corresponds to the bulk value for CdTe at $T = 77 \text{ K}$, while the 185-cm^{-1} line corresponds to an LO phonon in ZnTe layers “stretched out” to the CdTe lattice. The shift away from the bulk value $\omega_{LO} = 209 \text{ cm}^{-1}$ is $\Delta\omega = 24 \text{ cm}^{-1}$ and agrees fairly well with the calculated value $\Delta\omega = \Delta\omega_1 + \Delta\omega_2 = 24.8 \text{ cm}^{-1}$. Here $\Delta\omega_1 = 19.5 \text{ cm}^{-1}$ is the stress-induced shift, and $\Delta\omega_2 = 5.2 \text{ cm}^{-1}$ is the shift due to phonon localization. We should point out that we would have $\Delta\omega = 21.7 \text{ cm}^{-1}$ for a ZnTe phonon in the case of a free-standing configuration, and there should be a significant shift $\Delta\omega = 2.0 \text{ cm}^{-1}$ of the frequency of the CdTe phonon.

A comparison of the results of the present study with the results of Refs. 1 and 2 shows that the distribution of strain among the layers changes sharply, to a free-standing configuration, as the layer thickness is increased above d_c . We thus draw the qualitative conclusion that the stress relaxation occurs through the formation of a network of dislocations at the boundary between the superlattice and the buffer layer. The depth to which the dislocations penetrate into the superlattice would be anomalously small—only a few nanometers.

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