Superlattice Effects on Confined Phonons

In a recent Letter,[1] Sood, Menéndez, Cardona, and Ploog (SMCP) reported Raman measurements of confined LO and TO phonons in GaAs/AlAs superlattices. We focus on the results shown in Fig. 4 of SMCP, where the observed frequencies of the modes confined in GaAs layers deviate towards higher energy with respect to the folded bulk modes for $q \gtrsim \pi/a(100)$. In this Comment we show that this is a true superlattice effect; in fact, it is not explained in terms of an isolated slab calculation,[2] but can be accounted for by a model which treats properly both the superlattice geometry and the interatomic interactions.

We perform a calculation of the vibrational spectrum of the superlattice by representing it as a linear chain of (100) atomic planes[3] with *interplanar* force constants obtained[4] from an *ab initio* treatment of bulk GaAs within the local-density approximation. The same set of force constants is used for both materials, since it has been pointed out[5] that the different shapes of dispersion relations of III-V compounds are mainly due to different masses rather than to different bonding. This method is of striking simplicity and has the advantage of providing a very good description of the two bulks and of being easily applicable to superlattices of any thickness and composition.

In Fig. 1 we compare the calculated optical phonon frequencies of a $(GaAs)_7(AlAs)_7$ superlattice with the bulk ones; the agreement with the results of SMCP is remarkable. In particular, the effect of the superlattice marginally perturbs the TO modes at intermediate values of q, while it has a big effect on the LO close to the zone edge. The reason is that the confinement of LO modes becomes looser at large q as shown by the displacement pattern given in Fig. 2. Despite the fact that different modes have different decay lengths, the idea of confinement is still valid in that their displacements are mainly localized in one of the two materials and their frequencies do not depend on the thicknesses of the *adjacent* layers. However, the GaAs-like or AlAs-like modes have to be evaluated in the actual superlattice configuration. More detailed and comprehensive results will be presented in the future.

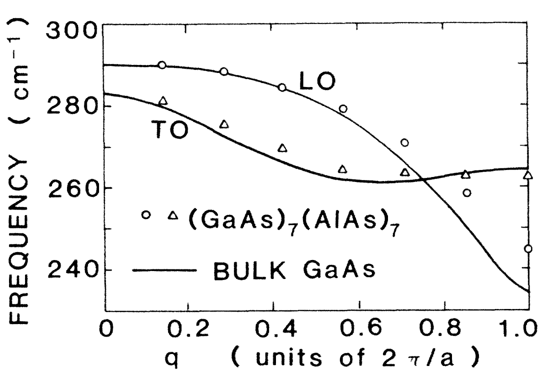

FIG. 1. Calculated GaAs-like LO and TO frequencies for the $(GaAs)_7(AlAs)_7$ (20 Å/20 Å) (100) superlattice as a function of $m\pi/d_{GaAs}$. Results for $(GaAs)_7(AlAs)_{21}$ are identical.

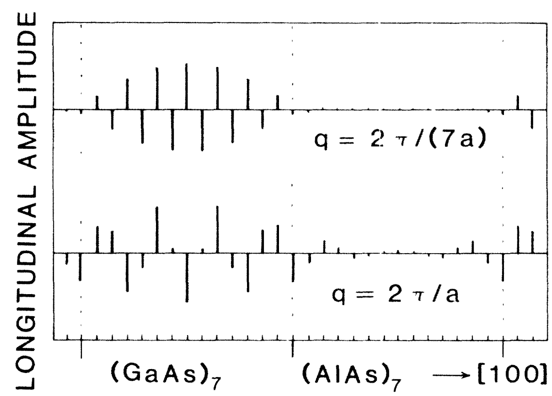

FIG. 2. Selected LO displacement patterns for $(GaAs)_7(AlAs)_7$ superlattice.

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