Elastic layered waves in (001) III-V nitride systems

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We have studied the acoustic waves in (001) single and multielastic wells formed by AlN, GaN, and InN in the zinc-blende structure. We have used the surface Green function matching method to obtain the dispersion relations and the local density of states. The anisotropy of the materials is included and the different propagation directions ranging from the [1,0,0] to the [1,1,0] have been considered. In these symmetry directions the sagittal waves are associated with a different velocity threshold than the transverse ones, thus showing a different behavior to that found in the isotropic case. For the [1,1,0] direction the sagittal modes are confined to a different range of velocities than the transverse modes. It has been found that the anisotropy introduces a more complex picture with a different mixing of the displacement components and the existence of different characteristics for different ranges of propagation direction.

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I. INTRODUCTION

The interest in surface and interface acoustic waves ranges from seismology[1] to ultrasonic processing devices,[2] with important applications to radar and communications,[3,4] passing through flaw detection[5] and quite recently to nanowave devices for terahertz acoustic phonons.[6] Many of the systems used now include one or several layers of different materials, which can be used for various purposes, such as to provide a desired dispersion characteristic,[7] as part of transducers for generating surface waves[8] or as a guiding region to confine a surface wave laterally.[9] Most of these systems use single crystals, thus making necessary the inclusion of the anisotropy in the theoretical studies. The cubic crystals are the simplest anisotropic systems and many of the materials of practical interest crystallize in the cubic system. It is then clear that layered structures formed by cubic crystals are the simplest ones to be considered.

In recent years the III-V semiconductor nitrides have shown an important potential for use in device applications. AlN, GaN, InN, and their ternary and quaternary alloys span an energy band gap range 1.9–6.2 eV, thus covering a potential color range from red to violet. These materials are suitable for surface acoustic wave devices,[10] UV detectors,[11–13] waveguides, UV, and visible light emitting diodes (LEDs) (Refs. 14–16) and laser diodes.[17,18]

These materials usually crystallize in the wurtzite structure, but it has been shown that they can be grown in the zinc-blende structure on different substrates.[19–29] There are some uncertainties concerning the data of zinc-blende GaN, AlN, and InN.[30] In particular, the elastic constants of these materials have not been determined experimentally until now. There are some theoretical calculations of the elastic constants of these materials. A calculation by using density-functional theory, *ab initio* pseudopotentials, and plane-wave expansions[31] can be taken as a representative, as shown in the study of the surface waves in these materials.[32]

These systems can serve to illustrate in a very general way the behavior of the acoustic waves in multilayer cubic systems including the anisotropy, that to our knowledge has not been considered.

Thus we shall study here the acoustic waves of (001) AlN, GaN, and InN layered systems. We shall use the surface Green function matching method[33] for systems with an arbitrary number (N) of interfaces[34] and we shall consider the different propagation directions ranging from the [1,0,0] direction to the [1,1,0] direction.

In Sec. II we give a brief description of the systems considered and the theoretical method. In Sec. III we discuss the results for the single and multielastic (001) wells. Conclusions are presented in Sec. IV.

II. THEORETICAL MODEL AND METHOD OF CALCULATION

We shall consider here the systems formed by one, three, and five material layers sandwiched between two semi-infinite blocks of the same material. In this way we can have situations similar to those of a single quantum well and multiple quantum wells. As we have noted before we shall concentrate on AlN, GaN, and InN layered systems. In Table I we give the mass density and elastic constants[31] of the zinc-blende AlN, GaN, and InN.

In cubic crystals a useful parameter is the anisotropy factor $[\eta=2C_{44}/(C_{11}-C_{12})]$. The velocity of a bulk transverse wave with its propagation vector in the (001) plane of a cubic crystal and polarized perpendicular to the plane is independent of the direction in this plane, whereas the velocity of the transverse wave polarized in the (001) plane increases if $\eta<1$, and decreases if $\eta>1$, with respect to that of the other transverse wave when the angle of propagation is rotated from the [1,0,0] to the [1,1,0] directions. We have $\eta(\mathrm{AlN})=2.680$, $\eta(\mathrm{GaN})=2.313$, and $\eta(\mathrm{InN})=2.774$.

Thus we must consider the velocities of the transverse waves, where for the [1.0,0] direction we have

$$c_{T2}=\sqrt{C_{44}/\rho}, \tag{1}$$

being doubly degenerate and for the [1,1,0] direction we have

$$c_{T1}=\sqrt{(C_{11}-C_{12})/2\rho}, \quad c_{T2}=\sqrt{C_{44}/\rho}. \tag{2}$$

TABLE I. Elastic constants calculated in Ref. 31 and mass densities employed in our calculations.

Material	$C_{11}(10^{10}$ N m$^{-2})$	$C_{12}(10^{10}$ N m$^{-2})$	$C_{44}(10^{10}$ N m$^{-2})$	$\rho(10^3$ kg m$^{-3})$
AlN	30.4	16.0	19.3	3.23
GaN	29.3	15.9	15.5	6.10
InN	18.7	12.5	8.6	6.81

It is easy to see that in our case $c_{T1}(\mathrm{AlN})=4.721$ km/s, $c_{T2}(\mathrm{AlN})=7.730$ km/s, $c_{T1}(\mathrm{GaN})=3.314$ km/s, $c_{T2}(\mathrm{GaN})=5.041$ km/s, $c_{T1}(\mathrm{InN})=2.134$ km/s, and $c_{T2}(\mathrm{InN})=3.554$ km/s. It is then clear that the velocities of the transverse waves in the InN are much lower than those in the GaN and the AlN. If the materials were isotropic the InN layer would load the GaN and AlN substrates, whereas the GaN layer would load the AlN substrate. In this case the phase velocities are reduced with increasing κD, D being the thickness of the layer.[35–37]

Then it is clear that we can consider that AlN acts always as a "barrier" and InN always as a "well." On the other hand, GaN would be a "well" versus AlN, but a "barrier" versus InN. It is then also clear that by combining these materials we can have polytype symmetric or asymmetric multielastic wells.

The surface Green function matching method[33] is especially suited to deal with multilayer systems.[34] The formal details of the method are given in Refs. 33 and 34 and here we shall give only the ingredients needed to study the (001) multilayer cubic systems.

We seek the Green's function $\mathbf{G}$ of the bulk material in Fourier transform with sign convention $\exp[i(\mathbf{k}\cdot\mathbf{r}-\omega\mathbf{t})]$. We consider $\mathbf{k}=(\boldsymbol{\kappa},q)$, where, in general, $\boldsymbol{\kappa}=(k_1,k_2)$. Then $\mathbf{G}(\mathbf{k},\omega^2)$ satisfies the equation

$$\sum_{m=1}^{3} L_{im}(\mathbf{k},\omega^2)G_{mj}(\mathbf{k},\omega^2)=\delta_{ij}, \tag{3}$$

where

$$L_{im}(\mathbf{k},\omega^2)=-\rho\omega^2\delta_{im}+C_{44}k^2\delta_{im}+(C_{12}+C_{44})k_ik_m + (C_{11}-C_{12}-2C_{44})k_i^2\delta_{im}. \tag{4}$$

Knowing $\mathbf{L}$ we evaluate

$$G_{ij}(\mathbf{k},\omega^2)=[L^{-1}(\mathbf{k},\omega^2)]_{ij} \tag{5}$$

by direct matrix inversion.

The surface projected elements of the Green function are obtained from

$$\mathcal{G}_{ij}(\boldsymbol{\kappa},\omega^2)=\lim_{\epsilon\to 0}\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp[i\epsilon q]G_{ij}(\boldsymbol{\kappa},q;\omega^2)dq, \tag{6}$$

whereas the normal derivatives are obtained from

$$'\mathcal{G}_{ij}^{(\pm)}(\boldsymbol{\kappa},\omega^2)=\lim_{\epsilon\to 0}\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp[\mp i\epsilon q]iqG_{ij}(\boldsymbol{\kappa},q;\omega^2)dq. \tag{7}$$

In the same way

$$G_{ij}(\boldsymbol{\kappa},x_3,x_3';\omega^2)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp[iq(x_3-x_3')]G_{ij}(\boldsymbol{\kappa},q;\omega^2)dq, \tag{8}$$

and

$$'G_{ij}(\boldsymbol{\kappa},x_3,x_3';\omega^2)=\frac{l}{\partial x_3}G_{ij}(\boldsymbol{\kappa},x_3,x_3';\omega^2). \tag{9}$$

From these projections and the boundary conditions at the different interfaces (continuity of the displacements and normal stress) we can obtain the interface projection of the Green function of the system $\tilde{\mathbf{G}}_S$.[34]

The dispersion relation is obtained by looking into the peaks of the density of states, which is obtained from the trace of $\tilde{\mathbf{G}}_S$.[34] The detailed expressions for all these elements can be easily obtained from those in Ref. 38.

III. RESULTS

We present here the results obtained for the multilayer systems formed with GaN and InN. The systems formed with the other combinations present a similar physical behavior and will not be presented here. The systems considered are GaN-InN-GaN (single well), GaN-InN-GaN-InN-GaN (double well), and GaN-InN-GaN-InN-GaN-InN-GaN (triple well). The GaN blocks at the extreme left and right sides are considered to be semi-infinite, whereas the thickness of the other layers is finite, the same for all of them and is taken as d. The total thickness D will be $D=d$, $D=3d$, and $D=5d$ for the single well, double well, and triple well, respectively. In the equivalent isotropic case all the modes would start from the semi-infinite media transverse threshold going asymptotically to the finite layer transverse threshold at large values of κD.

We have considered the cubic anisotropy in all the cases and obtained the dispersion relations for the different propagation directions including the symmetry [1,0,0] and [1,1,0] directions. In these directions the displacement component contained in the (001) plane is uncoupled from the other two forming the sagittal plane.[39,40] The situation is then formally analogous to that seen in the case of isotropic systems. On the other hand, in the remaining directions the modes exhibit a full coupling of the three displacement components and differences could be expected in the acoustic modes propagating in these general directions as compared to those propagating in the symmetry ones.

We have checked that no interface (Stoneley) waves[41] are present for any of the combinations of these systems. Thus we can have propagation only in the range of velocities con-

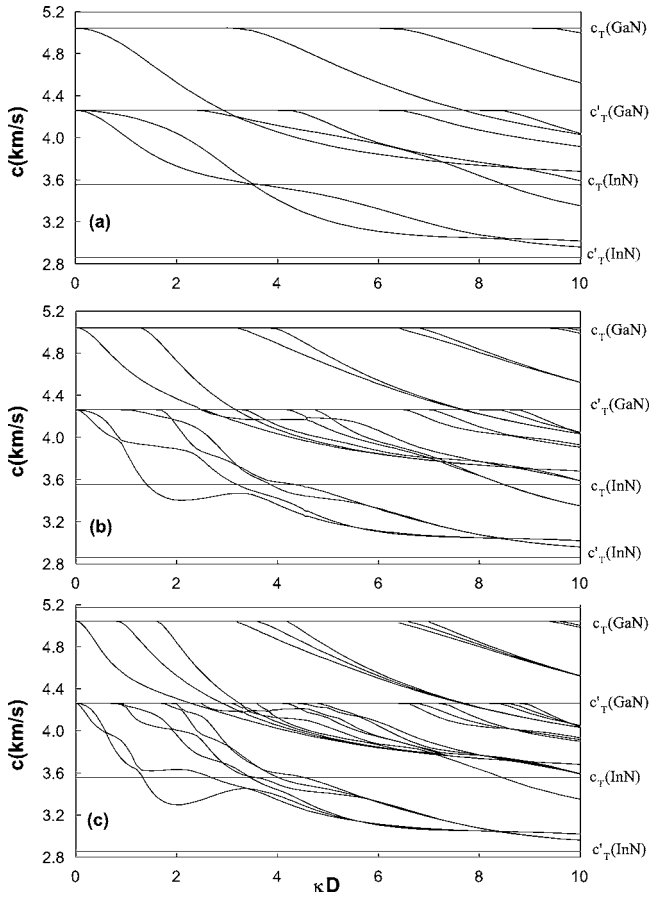

FIG. 1. Wave velocities in the [1,0,0] direction, as a function of κD for (a) the single well, (b) the double well, and (c) the triple well. The transverse waves exist in the range between the transverse threshold in GaN $[c_T(\mathrm{GaN})]$ and the transverse threshold in InN $[c_T(\mathrm{InN})]$. The sagittal waves exist between the thresholds $[c'_T(\mathrm{GaN})]$ and $[c'_T(\mathrm{InN})]$. For the meaning of these thresholds see the text.

tained between the lowest transverse waves of the two constituent materials.[35,42]

In Fig. 1 we present the wave velocities, in the [1,0,0] direction, as a function of κD for (a) the single well, (b) the double well, and (c) the triple well. The situation seen for the single well shows differences with respect to that found in isotropic materials.[35,42] It can be seen that we have waves coming from the transverse threshold in GaN $[c_T(\mathrm{GaN})]$, whereas we also have waves coming out from a velocity having a value $[c'_T(\mathrm{GaN})=4.261\ \mathrm{km\ s^{-1}}]$ between those of the transverse waves in GaN and InN $[c_T(\mathrm{InN})]$. We have checked by means of the contributions to the density of states that the modes coming from the GaN transverse threshold have purely transverse character with yy contributions, whereas the others exhibit a mixed character with xx and zz contributions. It is also clear that the sagittal modes cross the InN transverse threshold and tend aysmptotically to a different velocity. This behavior is different to that of the isotropic systems where these modes come from the transverse threshold of the semi-infinite medium and tend asymptotically to the transverse threshold of the finite layer.

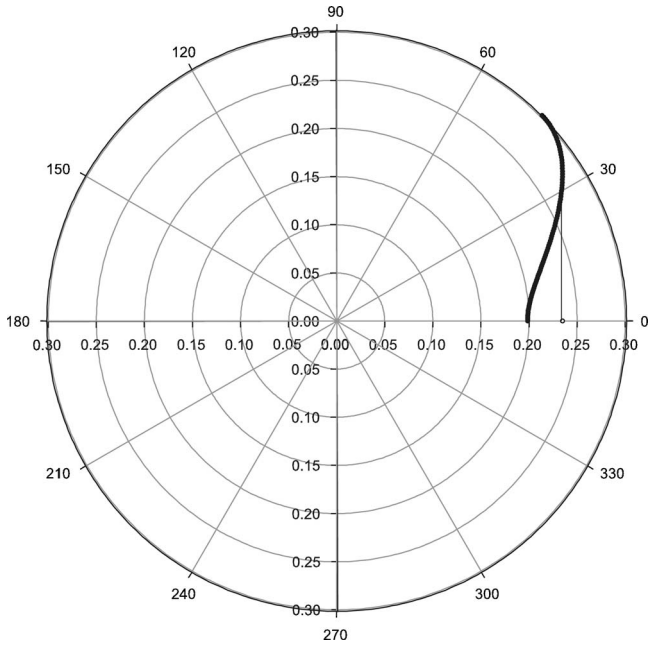

FIG. 2. Sagittal plane section of the slowness surface $1/c$ as a function of the angle of the propagation vector, for a bulk transverse wave in GaN.

We can understand the situation for the sagittal modes if we look to a sagittal plane section of the slowness surface $1/c$ as a function of the angle of the propagation vector, for a bulk transverse wave in GaN given in Fig. 2. For a bulk wave the direction of the Poynting vector is perpendicular to the slowness surface for each direction of the wave vector.[43] Thus it is seen that a bulk transverse wave with its propagation direction tilted ±32.3° to the (001) plane carries energy parallel to the (001) plane and the phase velocity measured parallel to this (001) plane is 4.261 $\mathrm{km\ s^{-1}}$, as indicated by the vertical straight line in Fig. 2.

This is also clear in Fig. 3 where we have represented the velocities of the different modes as a function of κD for an InN layer on a GaN substrate. We see that the transverse

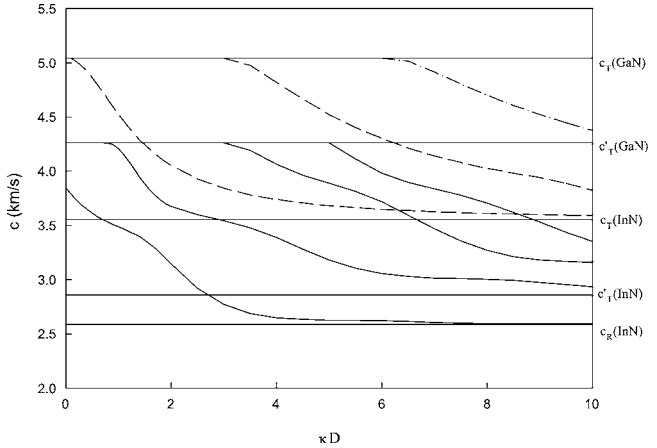

FIG. 3. Wave velocities in the [1,0,0] direction, as a function of κD for an InN layer on a GaN substrate. Transverse modes—dashed lines; sagittal modes—solid lines. For the meaning of the different thresholds see the text.

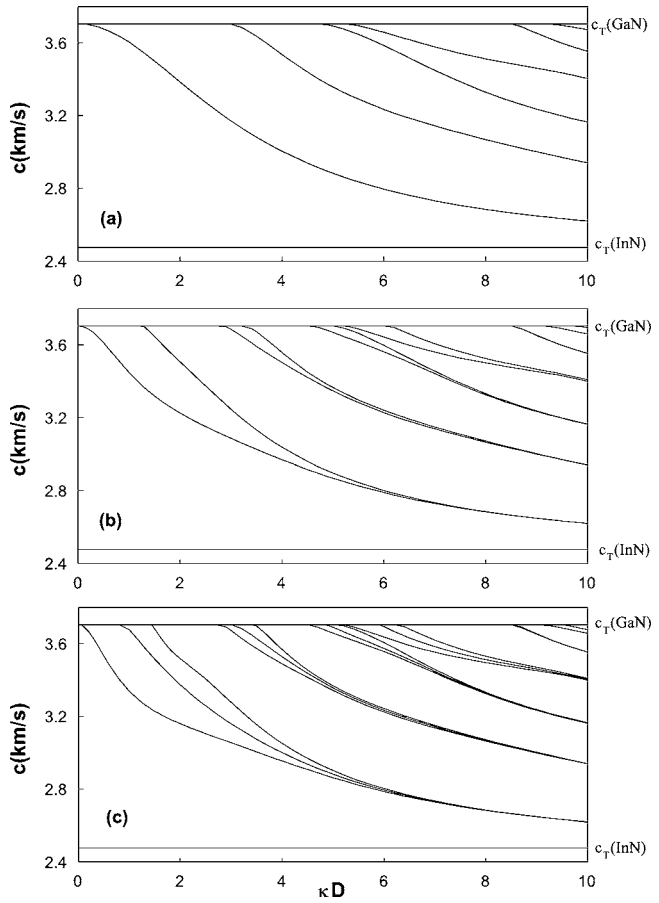

FIG. 4. As in Fig. 1 for the $\theta=30°$ propagation direction. All the branches are contained between the GaN slowest transverse wave $[c_T(\mathrm{GaN})]$ and the InN slowest transverse wave $[c_T(\mathrm{InN})]$.

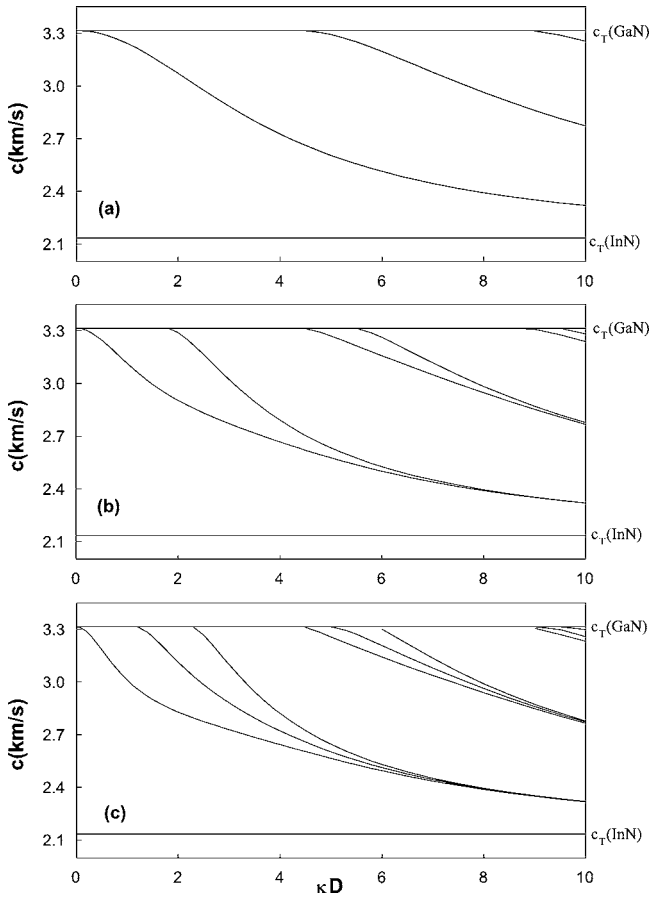

FIG. 5. Wave velocities of the transverse waves in the [1,1,0] direction, as a function of κD for (a) the single well, (b) the double well, and (c) the triple well. For the meaning of the different thresholds see the text.

modes (dashed lines) propagate in the region between the transverse thresholds of GaN $[c_T(\mathrm{GaN})]$ and InN $[c_T(\mathrm{InN})]$, whereas for the sagittal modes (solid lines) the first Rayleigh mode goes from the Rayleigh wave velocity in GaN to that in InN $[c_R(\mathrm{InN})]$, but the higher order Rayleigh modes show the same behavior seen in the well case coming from $c'_T(\mathrm{GaN})$ and tending asymptotically to a cutoff velocity in InN $[c'_T(\mathrm{InN})]$ having the same origin as that explained for GaN in Fig. 2. This is the behavior observed when both materials have the anisotropy factor $\eta>1$.[35] It is then clear that in the case of the well the first sagittal mode must come from the same origin than the higher order ones and that they will cross the InN transverse threshold instead of tending asymptotically to it, going instead to a different limit $[c'_T(\mathrm{InN})]$.

In the case of the double and triple wells the situation is similar to that of the single well but the number of branches is increased in a similar way to that of the electron states in multiple quantum wells. The results obtained here are quite similar to those experimentally observed in layered composites.[44]

The picture for propagation directions not close to the symmetry ones is represented in Fig. 4 for the propagation direction $\theta=30°$, θ being the angle formed by the propagation direction and the cubic x axis. The double and triple wells exhibit an increasing of the number of branches together with the splitting of some of them as in the case of the electron states in multiple quantum wells. In this case all the branches come from the GaN slowest transverse wave $[c_T(\mathrm{GaN})]$ and they tend asymptotically to the InN slowest transverse wave $[c_T(\mathrm{InN})]$. On the other hand, they have a mixed character with equivalent xx, yy, and zz contributions to the density of states. Those closer to the symmetry directions exhibit a picture more similar to these, and the coupling of the displacement components is lower in these cases.

In Fig. 5 we present the case of the transverse waves in the [1,1,0] direction, all of them having a yy contribution to the density of states. The behavior is in agreement with that seen for the transverse modes in isotropic systems. In Fig. 6 we present the dispersion relation for the sagittal modes. It is clear that they exist in the region between a cutoff velocity $[c'_T(\mathrm{GaN})]$ similar to that found in the [1,0,0] direction and the lowest GaN transverse threshold $[c_T(\mathrm{GaN})]$, where they tend in an asymptotic way. This shows a clear difference with the case of the isotropic media, where the transverse and sagittal modes are not confined to different ranges of existence. This situation can be understood when looking to the velocities of the different modes as a function of κD for an InN layer on a GaN substrate presented in Fig. 7. We see

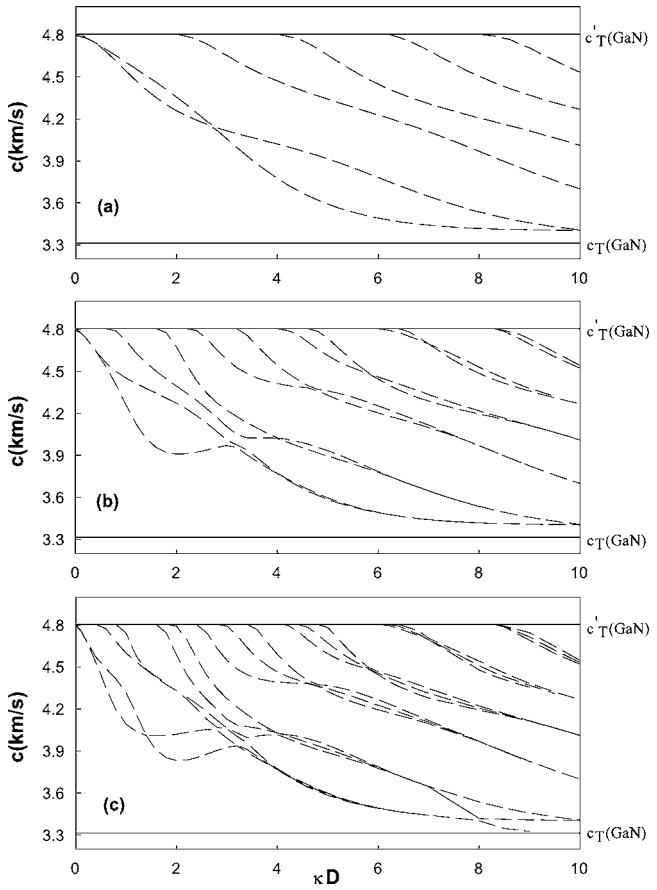

FIG. 6. Wave velocities of the sagittal waves in the [1,1,0] direction, as a function of κD for (a) the single well, (b) the double well, and (c) the triple well. For the meaning of the different thresholds see the text.

there all the transverse modes (solid lines) in the range between the lower transverse thresholds of GaN $[c_T(\mathrm{GaN})]$ and InN $[c_T(\mathrm{InN})]$, respectively. On the other hand, the sagittal waves (dashed lines) exhibit a different behavior. The first sagittal mode shows a velocity variation going from the velocity of the GaN pseudo-surface-wave $[c_{PSW}(\mathrm{GaN})]$ at $\kappa D=0$ to the InN pseudo-surface-wave $[c_{PSW}(\mathrm{InN})]$ at high κD. The higher order sagittal modes come from a cutoff velocity $[c'_T(\mathrm{GaN})]$ similar to the case of the [1,0,0] direction and have as the asymptotic limit the lowest GaN transverse threshold $[c_T(\mathrm{GaN})]$. Thus it is clear that with the existence of the well layer the sagittal modes will be restricted to a different range of velocities than the transverse modes. This behavior is quite different from that seen in the case of isotropic systems.

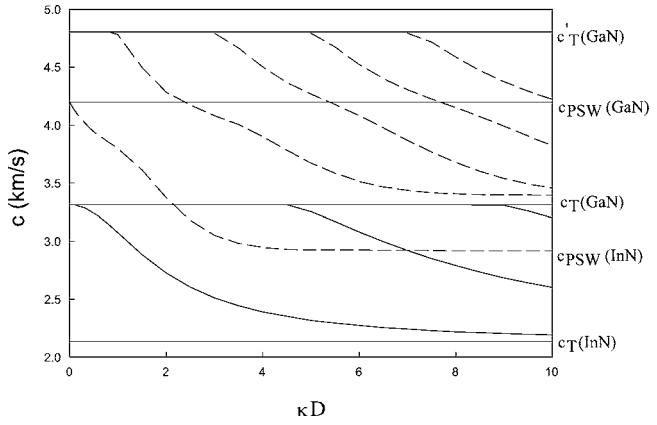

FIG. 7. Wave velocities in the [1,1,0] direction as a function of κD for an InN layer on a GaN substrate. Transverse modes—solid lines; sagittal modes—dashed lines. For the meaning of the different thresholds see the text.

For propagation directions near to the symmetry directions we obtain the same picture seen for the symmetry directions, although in this case all the waves have a mixing of the different components and they cannot be classified as sagittal or transverse.

The situation considered here is valid for all cubic systems having $\eta>1$ and the finite layer loading the semi-infinite media. Other possible combinations of anisotropy and material parameters would exhibit different behavior.

It is then clear that the anisotropy introduces a more complex picture with different mixing of the displacement components and the existence of different characteristics for different ranges of the propagation direction.

By looking to the evolution of the different branches when going from the single to the double and triple wells one can see the bunching together of these branches announcing the formation of the superlattice bands.

IV. CONCLUSIONS

We have studied the acoustic waves in (001) GaN/InN single, double, and triple elastic wells. Our results are valid for all cubic systems having $\eta>1$ and the finite layer loading the semi-infinite media. We have obtained the dispersion relations for the different propagation directions. In the [1,0,0] and [1,1,0] symmetry directions, due to the uncoupling of one transverse vibration, the situation is formally analogous to that found in isotropic materials but exhibit important differences. In both cases the sagittal waves are associated with a different velocity threshold than the transverse ones, thus showing a different behavior to that found in the isotropic case. For the [1,1,0] direction the sagittal modes are confined to a different range of velocities than the transverse modes. We have analyzed the case of a finite layer on a substrate in order to explain these behaviors. For propagation directions near to the symmetry ones we obtain the same picture seen for the symmetry directions, although in this case all the waves present a mixing of the different components and they cannot be classified as sagittal or transverse. For intermediate propagation directions we see a behavior similar to that of the isotropic case, with all waves going from the semi-infinite media transverse threshold to the finite layer transverse threshold in an asymptotic way, but now all the waves have a mixed character and cannot be classified as sagittal or transverse. The character of the different acoustic waves is also different for symmetry and arbitrary propagation directions as evidenced by the different contributions to the density of states.

We have seen that the anisotropy introduces a more complex picture with a different mixing of the displacement

components and the existence of different characteristics for different ranges of the propagation direction. In all the cases the double and triple wells exhibit more branches, in a similar way to the electron states in multiple quantum wells, and we can see in these branches the preliminaries of the superlattice bands.

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