

Strain effects on structural, dielectric, and lattice-dynamical properties of short-period GaN/AlN superlattices

J.-M. Wagner, J. Gleize,* and F. Bechstedt

Institut für Festkörpertheorie und Theoretische Optik, Friedrich-Schiller-Universität Jena

Max-Wien-Platz 1, D-07743 Jena, Germany

Fax: +49 - 36 41 - 94 71 52, e-mail: jmartin@ifto.physik.uni-jena.de

For GaN/AlN superlattices, one has a quite different physical situation compared to the case of GaAs/AlAs superlattices: first, the layers are mutually strained due to different lattice constants and there is an internal relaxation of the atomic layers at the interfaces, second, the optical phonon branches partially overlap, and third, the common anion is the lightest atom. Therefore, the use of IR reflectance or Raman spectroscopy for the characterization of the nitride heterostructures necessitates the knowledge of the special vibrational properties of the nitride superlattices and their strain dependence.

We investigate the strain influence on the structural, dielectric, and lattice-dynamical properties of short-period GaN/AlN superlattices by means of first-principles calculations. We consider both the cubic [001] and hexagonal [0001] structures. Within the framework of the density-functional theory, the local-density approximation and a plane-wave pseudopotential method, the effect of the Ga 3d electrons is also taken into account. The dielectric and vibrational properties are determined using the density-functional perturbation theory. To study the strain influence, we assume pseudomorphically strained layers and consider three different in-plane lattice constants corresponding to bulk AlN, bulk GaN, and an elastically relaxed average value.

For a given primitive cell of the superlattice, the internal degrees of freedom connected with the relaxation of the atoms near the GaN/AlN interface are treated by total energy minimization to obtain the relaxed structure, utilizing the Hellmann-Feynman forces for the atomic displacements. We obtain geometrical arrangements that differ from the ones predicted by macroscopic elasticity theory. From total energy calculations for strained structures, superlattices and bulk materials as well as ternary mixed crystals, we obtain the formation enthalpy which allows to determine the stability of the superlattice structures with different ordering of the layers.

Due to the strain-induced shift of the bulk phonon dispersions, the partial overlap of the LO branches of GaN and AlN is enhanced for the superlattices, giving an energetically separated region of all LO modes. In agreement with the picture of folded phonons, there exist LO modes that exhibit displacements of the nitrogen atoms only. The TO modes region is split into confined AlN and GaN phonons, with an interface mode reaching into the gap. Because of the opposite strain behaviour of the transversal acoustic phonons, their branch overlap is reduced and TA modes confined to the AlN layers occur.

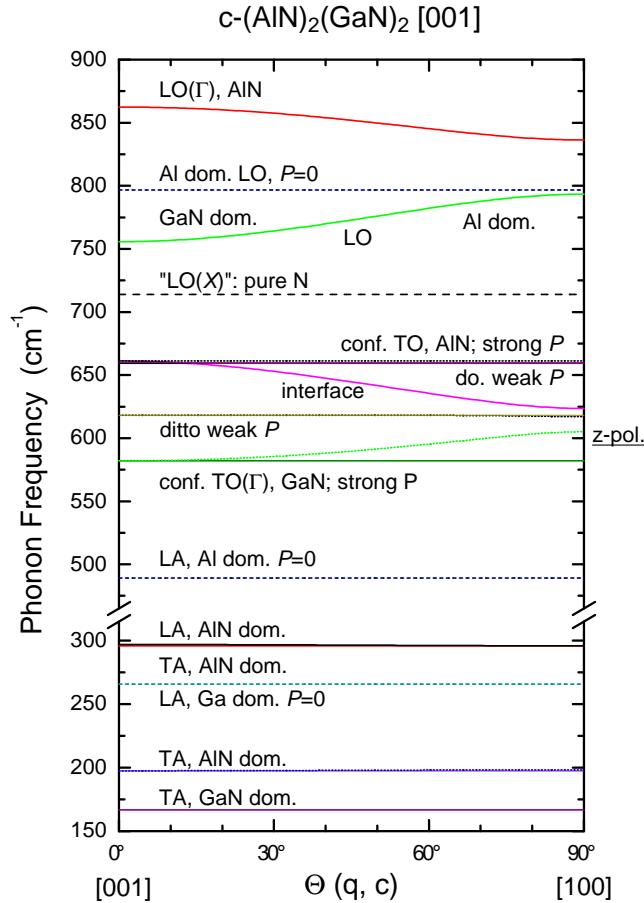
With increasing in-plane lattice constant, the optical modes and the folded LA modes decrease in frequency, whereas the folded TA modes shift to higher frequencies. This is completely analogous to the behaviour of the bulk materials under biaxial strain. For some adjacent acoustic modes of different kind the possibility of a reversed order of LA and TA modes is implied under different strain situations. There is a slight reduction of the gap between the TO modes, and in the cubic structures the downshift of the LO modes is more pronounced than that of the TO phonons.

Our particular interest concerns the angular dependence of the Γ -point phonon modes which helps to characterize the influence of the interfaces. All transversal phonons split into a dispersionless transversal and an angular-dependent mode with a mixed polarization, with the exception of an IR-active mode which exhibits angular dispersion despite of its TO nature. The angular dispersion of the interface mode in the TO-gap region is nearly independent of strain. The variation of the angular dependence with strain, i. e. the frequency difference for vertical and in-plane propagation, is stronger in the superlattices based on cubic crystals and most pronounced for the IR-active modes (highest LO mode and corresponding TO

* Permanent address: Laboratoire de Physique des Solides, Université Paul Sabatier, 118 route de Narbonne, 31062 Toulouse cedex 04, France

mode). This is due to a variation of the dynamical dipole moment P accompanying the vibration. In the compressive case of the AlN in-plane lattice constant, this variation is large and the splitting between the TO and the LO mode depends strongly on the angle, giving a pronounced angular dispersion of the LO mode. For the tensile GaN in-plane lattice constant, the dynamical polarization is nearly constant and the LO mode shows significantly less dispersion.

The similarities and differences to the case of superlattices with thicker material layers are discussed in terms of the macroscopic dielectric continuum model.



Angular dispersion of the Γ -point phonon modes of a "cubic" (tetragonal) $(\text{GaN})_2(\text{AlN})_2$ [001] superlattice. Θ denotes the angle between the c -axis of the superlattice and the phonon propagation direction \vec{q} . The labeling " P " refers to the dynamical dipole moment, $\vec{P} = \sum_{\kappa=1}^N \mathbf{Z}_\kappa^B \cdot \vec{u}_\kappa$ (N : number of atoms in the primitive cell, \mathbf{Z}_κ^B : tensor of the Born effective charge, \vec{u}_κ : vibration amplitude). The part of the superlattice (GaN or AlN) where each vibration dominates is indicated. For Θ approaching 90° , the dispersive GaN-confined TO mode involves both Ga and Al vibrations and is polarized in z direction, i.e. the atomic displacements are along the c -axis.