Raman spectra of short-period $(GaN)_n(AlN)_m$ superlattices: *ab initio* study

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The lattice dynamics and structural properties of short-period $(AlN)_m(GaN)_n$ ($m+n=4, 8, 12$ monolayers) superlattices (SLs) grown by MOVPE and PA MBE on the (0001) Al_2O_3 substrate are studied both theoretically and experimentally. The genesis of the SL phonon modes from the modes of bulk AlN and GaN crystals is established by applying a comprehensive group-theoretical analysis. The lattice dynamics is studied by *ab initio* calculations within the framework of the density functional theory. The dynamical matrix for a set of SLs is calculated within density functional perturbation theory (DFPT) and phonon eigenvalues and eigenvectors at the Γ-point of the Brillouin zone (BZ) are obtained. The eigenvectors analysis is performed to establish the irreducible representation of each vibrational mode. The number and symmetry of vibrational modes in the calculated phonon spectra are in complete agreement with the results of the group-theoretical analysis.

The Raman tensor components are calculated within DFPT and the theoretical Raman spectra are simulated and compared with experimental ones. The results of the *ab initio* calculations are in a good agreement with the experimental Raman data. The microscopic nature of the SLs vibrational modes is established by complex analysis of the results obtained both theoretically and experimentally. It is revealed that the phonon spectrum of GaN/AlN SLs is composed by mainly two types of phonon modes (localized and delocalized). It is found that the E(TO) modes are localized in the constituent SL layers and can be used to obtain information about the individual characteristics of each layer forming the SL. It is shown that the localized nature of the mode of this symmetry is preserved even in the SL with the thinnest constituent layers, i.e. for m+n=4. In turn, the A_1(TO) mode has a delocalized nature. This allows one to use the parameters of this mode to estimate the averaged characteristics of the SL as a whole. The correlation dependencies between the SL structure and the frequencies of the confined and delocalized polar phonons are obtained. The results of the study form the basis for the quantitative estimation of both strain in individual layers forming the SL and the Al(Ga) content averaged over the SL period. They also open new possibilities for the analysis other important parameters of short-period GaN/AlN SLs.

The work is supported by Russian Science Foundation Project (Grant No. 19-72-30040).