Lattice Dynamics of the Zinc-Blende and Wurtzite Phases of Nitrides

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An adiabatic bond charge model has been applied to calculate the phonon dispersion and the density of states of the nitride materials BN, AlN, GaN and InN in the zinc-blende and wurtzite phases. It is found that the results obtained from the application of this phenomenological theory for lattice dynamics compare very well with available experimental measurements and with recent *ab inito* calculations [1,2]. From our work we estimate the width of the angular dispersion of the zone-centre Raman active A_1(LO)–E_1(LO) branch in the wurtzite phase to be 40 cm^{-1}, 10 cm^{-1} and 3 cm^{-1} for AlN, GaN and InN, respectively. These results are linked to the trend in the Phillips ionicity of these materials. The crystal anisotropy factor $[\omega_{\rm TO}(E_1,\Gamma)-\omega_{\rm TO}(A_1,\Gamma)]/\omega_{\rm TO}(E_1,\Gamma)$ is calculated to be 0.04, 0.02 and 0.02 for AlN, GaN and InN, respectively. This indicates, in complete agreement with a recent *ab initio* work [3] that AlN is more anisotropic than GaN and InN. We also find that the anticrossing behaviour of the A_1 acoustic and E_2 optical modes takes place at approximately 0.9Γ-K in the Brillouin zone. Finally, we briefly discuss the spontaneous three-phonon decay of the zone-centre LO phonon in these materials and their alloys.

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