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Title:Thermal expansions in wurtzite AlN, GaN, and InN: First-principle phonon calculations

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Abstract:Using the first-principle phonon calculations under the quasiharmonic approximation, thermal expansions in III-nitrides with wurtzite AlN, GaN, and InN are reported. The results showed that it is different for each thermal expansion of three III-nitrides at low temperatures, which is consistent with their Grneisen parameters as the function of temperature. Below 50 K, negative thermal expansions occur in InN, while GaN and AlN follow the rule of positive thermal expansion. To seek the origin of positive/negative thermal expansion distinction, the mode Grneisen parameters and the phonon spectra are investigated. They indicate that different low-frequency phonon vibration modes correspond to the change of thermal expansions. Below 5 THz, the significant weighted negative values of mode Grneisen parameters, caused by the weakening of mixing-mode constituted with two transverse acoustic (TA) modes and a small overlapped part of optical modes, directly lead to the negative thermal expansion at low temperatures. © 2011 American Institute of Physics.