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First-principles phonon calculations as a method of improving the atomistic thermodynamics of III-nitrides surfaces

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In this paper, we would like to show how phonon calculations can be used to improve the thermodynamic description of III-nitride surfaces in the context of growth by epitaxial methods. Theoretical atomistic analysis of the system representing the crystal surface in contact with the gas phase are often performed. In particular, density functional theory (DFT) calculations are leading method in this field. Unfortunately, this method describes the system at the temperature of absolute zero. In the standard approach of atomistic thermodynamics, the free energy of the vapour phase at a given temperature is considered, whereas the surface is described by the total energy determined on the basis of DFT calculations at 0˚K. Phonon calculations can be successfully used to improve the accuracy of this theoretical model. Recently, we presented such an analysis that more accurately describes the hot GaN surface under growth conditions [1]. We included a contribution derived from thermal vibrations determined on the basis of phonon calculations for slabs representing the surface. In this way, several temperature-dependent properties of surface, such as vibrational energy and vibrational entropy can be determined. The thermal dependence of surface free energy was included in predicting the evolution of surface reconstruction under growth conditions, and thus the phase diagrams of the GaN(0001) surface were improved. The example of hydrogen adsorption on the GaN(0001) surface has shown that adding of accurate entropy contributions (vibrational and configurational) can significantly change the predicted equilibrium hydrogen pressure above the surface [2].

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Refs
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