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Towards High-Fidelity InGaN Interatomic Potentials

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ABSTRACT

To enable efficient green light emission for solid-state-light applications, the indium content x in the $In_xGa_{1-x}N$/GaN multilayers must be high. However, increasing indium content increases lattice mismatch, which in turn causes performance deterioration due to strain relaxation and defect formation. To help increase indium content through nanostructuring experiments, molecular dynamics simulations of $In_xGa_{1-x}N$/GaN multilayers are useful. To enable such molecular dynamics simulations, we have been developing high-fidelity InGaN interatomic potentials. In a first step, we have developed an InGaN Stillinger-Weber potential. This potential captures well the lattice constant, cohesive energy, and elastic constants of the wurtzite GaN and InN. In particular, it reproduces exactly the experimental atomic volume, cohesive energy, and bulk modulus of GaN and InN. It also captures well the relative energy change between elements, alloys, and compounds so that direct molecular dynamics simulations can predict crystalline growth of both GaN and InN. Such a potential can be accurately used to study stoichiometric compounds. In a second step, we report our progress on developing a modified InGaN Stillinger-Weber potential that improves the prediction of atomic volume and elastic constants of elements so that the simulations can be accurate for non-stoichiometric conditions. Finally, we introduce a new polymorphic pair style that enables lammps molecular dynamics simulations to be applied for any modified potentials based on Tersoff, Stillinger-Weber, and embedded-atom method formats.

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