Abstract Submitted
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Short-range order and its effects on electrons in $(GaN)_{(1-x)}(ZnO)_x$ alloys[1] JIAN LIU, LUANA PEDROZA, Stony Brook University, CARISSA MISCH, Smith College, MARIA FERNANDEZ-SERRA, PHILIP ALLEN, Stony Brook University — Prior work by Li et al. gives "cluster expansion" parameters for $(GaN)_{(1-x)}(ZnO)_x$ alloys. From these, by Monte-Carlo calculations, large representative unit cells can be generated at any chosen temperature. We choose mainly T=1200K, typical of the temperature at which experimental samples fall out of equilibrium. The atoms are distributed on the wurtzite anion and cation sublattices with significant short-range order. A periodic supercell with 432 atoms is chosen as a compromise between accurate self-averaging and fully self-consistent and relaxed density-functional (DFT) computation. Composition- and temperature-dependent short-range order (SRO) parameters of the alloys are discussed. Entropy is related to the SRO parameters. DFT relaxation finds significant bond-length alterations. Typical Zn-O distances are larger by 10% than Ga-N distances in the alloy, even though in pure ZnO and GaN, bond lengths are nearly equal. Electronic properties of the alloys, and in particular, the influences of short-range order and bond-length fluctuations, will be discussed.

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