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The influence of the lattice relaxation on the optical properties of GaN_xAs_{1-x} alloys

Abstract

We have investigated the optical properties of the ternary alloys GaN_xAs_{1-x} (x=0.25, 0.5 and 0.75) without (we call it as case 1) and with (case 2) the lattice relaxation, using the full potential-linearized augmented plane wave (FP-LAPW) method. The exchange-correlation contribution was described within the generalized gradient approximation (GGA) proposed by Perdew et al. to calculate the total energy, while for electronic properties in addition to that the Engel-Vosko (EVGGA) formalism was applied. In case 1, we have only optimized the lattice constant without relaxing the atomic positions, whereas in case 2 we have relaxed the atomic positions to find the equilibrium atomic configurations. The alloys were modeled at some selected compositions x=0.25, 0.5 and 0.75 following the 'special quasirandom structures' (SQS) approach of Zunger to reproduce the randomness of the alloys for the first few shells around a given site. For relaxed alloys, the lattice constants vary linearly as function of composition x however, if internal relaxation is not allowed, significant deviations from Vegard's law occur. In general the imaginary part of the dielectric function of the two cases for each compositions look similar at the high energies while there is significant differences at the low energies. The reflectivity spectra, electron energy loss function and absorption coefficient are also calculated and analyzed. Taking in consideration the lattice relaxation effect, the results are more reliable.

Keywords — Ab initio calculations, GaN_xA_{1-x} alloys, optical properties, semiconductivity