Structural, optoelectronic, and thermodynamic properties of $Y_xAl_{1-x}N$ semiconducting alloys

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Abstract

The structural, electronic, optical, and thermodynamic properties of $Y_xAl_{1-x}N$ alloys were computed using first-principles calculations. The effects of exchange and correlation have been considered by means of the generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof parametrization. In addition, the Tran–Blaha-modified Becke–Johnson potential (TB-mBJ) was applied to give a better description of the band-gap energies and optical spectra. The lattice parameters, bulk modulus, and band-gap energy show nonlinear dependence on concentration x. Results for rock-salt $Y_xAl_{1-x}N$ alloys show that the band gap undergoes an indirect (Γ→X)-to-direct (Γ→Γ) transition at a given yttrium composition, followed by a direct (Γ→Γ)-to-indirect (Γ→X) transition in a higher yttrium concentration. For wurtzite $Y_xAl_{1-x}N$ alloys, the band gap presents a direct (Γ→Γ)-to-indirect (→Γ) transition at a given yttrium composition, followed by an indirect (→Γ)-to-indirect (M→Σ) transition in a higher yttrium concentration. The real dielectric function, imaginary dielectric function, refractive index, and extinction coefficient were calculated using the TB-mBJ potential. Using a regular solution model, slightly lower mixing enthalpies for wurtzite $Y_xAl_{1-x}N$ alloys were found. The mixing enthalpy for a given concentration differs depending on structures, and on the interaction between atoms of constituents. The effect of temperature on the volume, bulk modulus, Debye temperature, and the heat capacity for $Y_xAl_{1-x}N$ alloys was analyzed using the quasi-harmonic Debye model. Results show that the heat capacity is fairly sensitive to composition as temperature increases.

Keywords

Bulk Modulus, Wurtzite, Dielectric Function, Wurtzite Phase, Yttrium Concentration