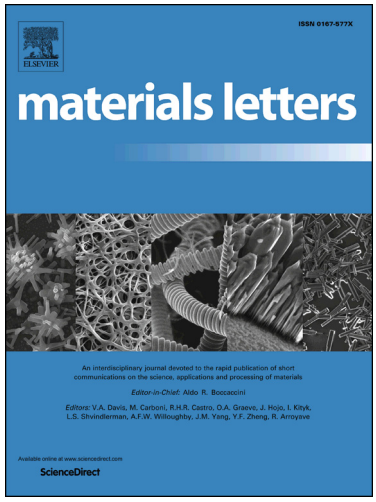

First-principle survey of structural, electronic, and optical properties of zinc-blende $B_xAl_yGa_{1-x-y}N$ quaternary alloy

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First-principle survey of structural, electronic, and optical properties of zinc-blende $B_xAl_yGa_{1-x-y}N$ quaternary alloy.

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Abstract

We present first-principle calculations of structural, electronic, and optical properties of zinc-blende (z) $B_xAl_yGa_{1-x-y}N$ quaternary alloy, using alchemical mixing of plane-wave pseudopotentals method based on density functional theory (DFT). Generalized gradient approximation (GGA) is used to describe exchange-correlation potential coupled with the Perdew, Burk and Ernzerhof (PBE) flavour. The calculated structural properties, equilibrum lattice constant and bulk modulus are in excellent agreement with available theoretical and experimental data. The bandgaps obtained depend on alloying concentrations x and y. The bandgap and density of states (DOS) are in good agreement with available theoretical data. The optical spectra obtained are given in the energy range of 0-8eV. The results obtained in this calculation indicate that $z - B_xAl_yGa_{1-x-y}N$ alloy is a desirable material for manufacturing of deep ultraviolet (UV) light emitting diodes (LEDs) and laser diodes (LDs).

Keywords: first-principle; structural; electronic; optical; quaternary alloy; zinc-blende

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