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Novel BTlGaN Semiconducting Materials for Infrared Opto-Electronic Devices

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Abstract

BTlGaN quaternary alloys are proposed as new semiconductor materials for infrared opto-electronic applications. The structural and opto-electronic properties of zinc blende $B_xTl_yGa_{1-x-y}N$ alloys lattice matched to GaN with ($0 \leq x$ and $y \leq 0.187$) are studied using density functional theory (DFT) within full-potential linearized augmented plane wave (FP-LAPW) method. The calculated structural parameters such as lattice constant a_0 and bulk modulus B_0 are found to be in good agreement with experimental data using the new form of generalized gradient approximation (GGA-WC). The band gaps of the compounds are also found very close to the experimental results using the recently developed Tran–Blaha-modified Becke–Johnson (TB-mBJ) exchange potential. A quaternary $B_xTl_yGa_{1-x-y}N$ is expected to be lattice matched to the GaN substrate with concentrations x= 0.125 and y= 0.187 allows to produce high interface layers quality. It has been found that B incorporation into BTlGaN does not significantly affect the band gap, while the addition of dilute Tl content leads to induce a strong reduction of the band gap, which in turn increases the emission wavelengths to the infrared region. The refractivity, reflectivity and absorption coefficient of these alloys were investigated. BTlGaN/GaN is an interesting new material to be used as active layer/barriers in quantum wells suitable for realizing advanced Laser Diodes and Light-Emitting Diodes as new sources of light emitting in the infrared spectrum region.

Keywords: BTlGaN quaternary alloy, Laser Diodes, Lattice-matching, TB-mBJ functional, Opto-Electronic properties.

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