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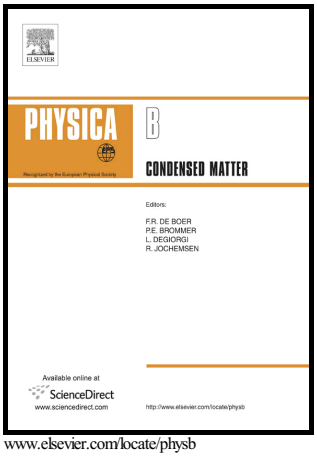

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Structure, electronic and mechanical properties of $Ga_{1-x}B_xP$ alloys

Bin Zhao[1], Junqin Zhang[1*], Huihui Ma[1], Qun Wei[2], Yintang Yang[1]

[1]*Key Laboratory of Ministry of Education for Wide Band Gap Semiconductor Materials and Devices, School of Microelectronics, Xidian University, Xi'an 710071,China;*

[2]*School of Physics and Optoelectronic Engineering, Xidian University, Xi'an 710071,China;*

[*]*Correspondence: Tel.: +86-29-8820-2579. zhangjq@mail.xidian.edu.cn*

Abstract

The structural, electronic and mechanical properties of $Ga_{1-x}B_xP$ ternary alloys are carried out by the first-principles based on density functional theory. We studied the effect of composition on the ground state properties such as lattice parameter, band gap and elastic modulus and anisotropy. The elastic anisotropy of $Ga_{1-x}B_xP$ alloys have been described through different anisotropic factors. We analyzed elastic anisotropy by depicting the three-dimensional surface structure of elastic modulus. Due to the introduction of boron atoms, the $Ga_{1-x}B_xP$ alloys become direct-gap semiconductors at x = 0.25, 0.50 and 0.75. At last, we calculated the average acoustic velocity in different directions and the Debye temperatures for the $Ga_{1-x}B_xP$ alloys.

Keywords: $Ga_{1-x}B_xP$ alloys; Electronic properties; Band structure calculations; Mechanical properties;