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# DIELECTRIC CONSTANTS AND TRANSVERSE EFFECTIVE CHARGES IN THE QUINARY ALLOY $Ga_xIn_{1-x}N_ySb_zAs_{1-y-z}$ LATTICE MATCHED TO InAs, GaSb AND GaAs

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This study provides a comprehensive theoretical analysis of the dielectric properties and transverse effective charges of the pentanary alloy $Ga_xIn_{1-x}N_ySb_zAs_{1-y-z}$, focusing on compositions that are lattice-matched to InAs, GaSb, and GaAs substrates. The investigation employs the local empirical pseudopotential method (EPM) in conjunction with the virtual crystal approximation (VCA) and the Harrison bond-orbital model to evaluate key parameters, including the static and high-frequency dielectric constants, ionicity, polarity, and transverse effective charge. These computational approaches were chosen due to their ability to accurately describe electronic interactions in complex alloy systems while maintaining computational efficiency. The results demonstrate strong consistency with available experimental data for the constituent binary compounds, reinforcing the reliability of the theoretical framework. Additionally, the study reveals systematic trends in the dielectric behavior as a function of composition, providing insights into the role of atomic substitution in tuning these properties. To the best of our knowledge, this work represents the first detailed theoretical assessment of $Ga_xIn_{1-x}N_ySb_zAs_{1-y-z}$ alloys in this context. While experimental validation remains necessary, our findings establish a valuable theoretical benchmark for future studies and potential applications in optoelectronic and semiconductor device engineering, particularly in the design of advanced infrared detectors and high-frequency electronic components.
**Keywords:** *EPM; Polarity; Dielectric constants; Transverse effective charge; Lattice matched alloys; Pentanary*
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## 1. INTRODUCTION

The integration of III-N-V semiconductors into modern optoelectronic and high-frequency microelectronic devices has gained significant attention due to their unique electronic and optical properties [1]. These materials exhibit direct band gaps [2], high carrier mobilities, and tunable electronic characteristics, making them essential for applications such as infrared photodetectors, laser diodes, and high-speed transistors [3,4]. In particular, they are widely used in fiber-optic communication systems, where the 1.3 μm and 1.5 μm wavelength regimes are critical for minimizing signal attenuation [5]. The incorporation of nitrogen into III-V semiconductors plays a crucial role in band gap engineering, as even small amounts of nitrogen induce a substantial reduction in the band gap [6], thereby allowing for precise control of optical and electronic properties.

Among the various III-N-V compounds, the pentanary alloy $Ga_xIn_{1-x}N_ySb_zAs_{1-y-z}$ presents a promising material system with highly tunable properties while maintaining lattice-matching conditions with widely used substrates such as InAs, GaSb, and GaAs. Ensuring lattice matching is essential for epitaxial growth, as strain-induced defects can significantly degrade the material's electronic transport properties, optical efficiency, and thermal stability. The ability to engineer the band gap and dielectric properties of pentanary alloys while preserving structural compatibility with established semiconductor platforms opens new avenues for the development of advanced optoelectronic devices. Despite their technological potential, pentanary III-N-V alloys remain largely unexplored in terms of their dielectric response and transverse effective charge behavior. While binary and ternary III-V semiconductors have been extensively studied, the complexity introduced by five constituent elements makes direct experimental characterization particularly challenging. This necessitates a rigorous theoretical investigation to systematically analyze the dielectric properties of $Ga_xIn_{1-x}N_ySb_zAs_{1-y-z}$, providing critical insights that can serve as a theoretical foundation for experimental studies and device optimization.

To achieve an accurate and predictive description of the dielectric properties of these alloys, we employ a combination of well-established theoretical approaches. The local empirical pseudopotential method (EPM) is utilized to model electron-ion interactions, providing an effective means of describing the electronic band structure of complex multi-component alloys [7,8]. This method has been extensively validated against experimental data for binary III-V semiconductors, demonstrating its reliability in capturing essential electronic properties. The virtual crystal approximation (VCA) [9] is employed to treat the pentanary alloy as an effective medium, where the electronic properties are approximated as a weighted average of the constituent binaries. This approximation offers a computationally efficient means of estimating key dielectric parameters, ionicities, and transverse effective charges, enabling a predictive framework for understanding composition-dependent variations in material properties. Additionally, Harrison's bond-orbital model [10,11] is incorporated to refine the description of chemical bonding, interatomic interactions, and charge transfer effects. This analytical approach allows the

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