

Theory of Idealized and Imperfect Antimonide-Based Superlattices.

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We present the results of a series of optical and dynamical calculations carried out on antimonide-based superlattice systems. We employ band structure and carrier scattering models describing the atomic potentials in both idealized and disordered heterostructure systems. These enable us to establish quantitative links between the microscopic interface signature and those properties which govern the characteristics of potential devices.

If the antimonides are to be taken on board by optoelectronics manufacturers as alternatives to standard material systems in infrared applications, such as GaAs/AlGaAs, a quantitative understanding of the relationships between the atomistic features of these systems and the key device performance parameters must be achieved. Specifically, to improve the characterization and understanding of these systems, knowledge of the physics linking disorder and interface distortion with carrier scattering and the optical properties is required. This would enable designers to anticipate the properties and limitations of these systems in proposed technological applications.

In this paper, we report several series of calculations which probe these issues in GaSb/InAs-based superlattice systems. We investigate the effects which the heterojunction bond types have on the band gap, wave functions and absorption spectra in idealized (that is, disorder-free) superlattices. We predict some significant differences in these parameters for the various interface type combinations, suggesting that control of the shutter sequencing during epitaxy is paramount. Studies of alloy layer disorder also indicate some interesting consequences for emission processes. Additionally, carrier scattering resulting from isovalent defects, as have been found to arise from cross-interface diffusion during fabrication, has been modeled for these systems. We investigate the dependence of the scattering cross-section on the position of isolated anion and cation defects in the unit cell. The relationship between the cross-section and the size of clusters of such defects is also studied. Some interesting non-linearities in the cross-section were observed when modeling islands of anion defects surrounded by isolated cation defects in adjacent layers.

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