A Comprehensive Modeling Approach of Electronic Properties in III-V Digital Alloys

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***Abstract*—We employ an Environment-Dependent Tight Binding Model and a band unfolding technique to study the effect of strain in III-V digital alloys. Furthermore, we employ the Non-Equilibrium's Green's Function formalism and a Boltzmann transport solver to study the carrier transport in these digital alloys.**

I. Introduction

In recent times, avalanche photodiodes (APDs) are becoming the preferred photodetector in applications like single photon detection, fiber optic communication and LIDAR systems. APDs are favored over p-i-n photodiodes due to their low noise and high gain-bandwidth product. The stochastic nature of the impact ionization process in APDs leads to an additional excess noise. The excess noise factor given by, $F(M) = kM + (1-k)(2-1/M)$, is directly proportional to the ratio of ionization coefficients $k = \beta/\alpha$ [1]. Here, β is the hole ionization coefficient and α is the electron ionization coefficient. By making one of the ionization coefficients greater than the other it is possible to reduce the excess noise factor. Recently, some III-V digital alloy APDs have demonstrated such low excess noise [2-4]. The low excess noise can be attributed to a combination of small minigaps in the valence band, higher valence band effective mass and a large separation between the light-hole and split-off bands. These properties localizes the holes and prevents them from gaining the ionization threshold energy. This makes β much less than α which results in a more deterministic multiplication process that reduces the excess noise.

In this paper, we particularly look at the role of minigaps in reducing the excess noise in APDs. We explain how biaxial strain leads to the formation of these minigaps using an environment-dependent tight binding model. Furthermore, we employ a ballistic Non-Equilibrium's Green Function (NEGF) model and a Boltzmann Transport solver to study the effect of these minigaps on carrier transport in the digital alloys. Based on simulations using the aforementioned tools we show that biaxial contraction can result in larger minigaps which can potentially reduce the noise in digital alloy APD structures.

II. Results and Discussion

In digital alloys, binary compounds are assembled on top of each other in a periodic manner as shown in Fig. 1. In the case of a 6-monolayer InAlAs digital alloy grown on an InP substrate, InAs and AlAs are stacked alternately. The bandstructure for these digital alloys are computed using the Environment-Dependent Tight Binding (EDTB) Model [5]. Traditional tight binding model is calibrated to bulk bandstructure and cannot be easily transferred to surfaces or interfaces as their chemistry is significantly influenced by their environment. The parameters in the traditional models cannot be readily adjusted, as these work directly in conjunction with eigenvalues and not the full eigenvectors, whose radial parts are especially important for bonding and tunneling. On the contrary, the EDTB model includes orthogonal Wannier like basis sets, and is calibrated to Density Functional Theory (DFT) wavefunctions as well as DFT bandstructure. State-of-the-art Hybrid (HSE06) functional are used to compute the DFT bandstructure and wavefunctions which match experimental results accurately. Thus, the EDTB model is able to accurately incorporate the material chemistry at the interfaces/surfaces. The bandstructure of strained InAs and AlAs is shown in Fig. 2(a).

Large unit cells are needed to compute the bandstructure of superlattice structures like digital alloys. This results in a complicated bandstructure which does not provide significant insight. Consequently, we employ a band unfolding technique to simplify the digital alloy bandstructure. This method involves projecting the bands of the smaller supercell Brillouin zone onto the large Brillouin zone of the bulk primitive cell of its pristine binary components [2,6]. Fig. 2(b) depicts the unfolded bandstructure of a 6-monolayer InAlAs digital alloy grown on InP. We observe small gaps opening up in the InAlAs light-hole band called minigaps. The bands near the minigaps are also flattened as a result, leading to an increase in effective mass. These minigaps and increased mass together confine holes near the valence band edge and prevent them from gaining ionization threshold energy. As a result, the hole ionization coefficient of InAlAs reduces significantly, leading to low excess noise in APDs. Since biaxial strain results in the formation of minigaps we can tune the strain to control the minigap size. We consider two cases: contraction- where the substrate lattice constant is lower than that of InP, and expansion- where the substrate lattice constant is greater than the InP lattice constant. The InAlAs bandstructure for the two

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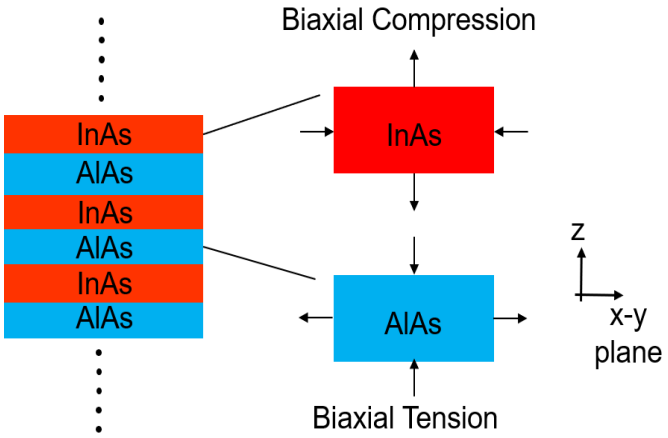

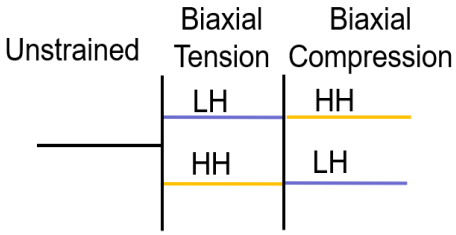

Fig. 1. InAs and AlAs stacked alternately in a 6-monolayer InAlAs grown on InP substrate. InAs experiences biaxial compression in the $x-y$ plane and AlAs experiences biaxial tension. Both these types of strain results in the splitting of the heavy-hole and light-hole bands.

cases is shown in Fig.3. We observe that minigap size increases under contraction.

It is possible to overcome the minigaps by two possible mechanisms- quantum tunneling and optical phonon scattering. We employ a ballistic NEGF model that utilizes the Hamiltonian from the EDTB model in order to study the quantum tunneling in the digital alloys. Usually, a real space DFT Hamiltonian, $H(x,y,z)$, is used for this purpose. This Hamiltonian is Fourier transformed in the $x-y$ plane to get $H(x,k_y,k_z)$ as structures are translationally invariant in the $x-y$ plane. The 3D EDTB Hamiltonian, which is in k-space basis, is inverse transformed to generate hopping elements along the transport direction [7] to obtain a quasi-1D Hamiltonian. Then, we use the Fisher-Lee formula in NEGF to compute the energy dependent transmission in the valence band for the three cases of InAlAs considered above, under bias. The transmission plots are shown in Fig. 4(a) and we can see there that there are large transmission gaps with increasing minigap size. To go beyond ballisticity, we use a Boltzmann transport solver to compute the energy resolved carrier occupation probability in the valence band to study the effect of optical phonon scattering in these alloys. We derive an effective constant scattering strength from experimental mobility to compute the optical phonon scattering rate using Fermi's Golden Rule. The simulated results from the Boltzmann transport calculations are shown in Fig. 4(b). We observe that with increasing minigap size the occupation probability at high energies in the valence band decreases. Together, these tools provide us with an efficient and accurate method to study the electronic properties of III-V digital alloys.

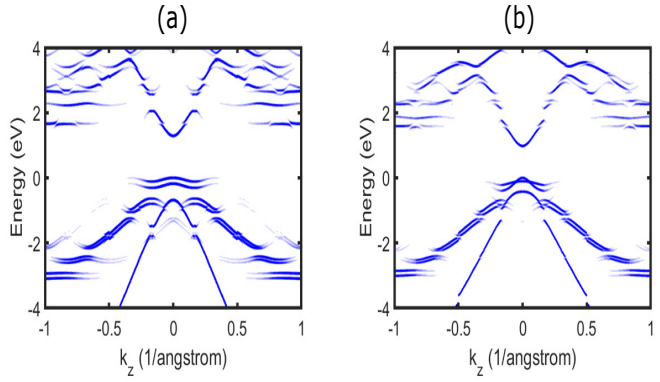

Fig. 3. (a) Bandstructure of strained InAs and AlAs that is grown on InP substrate (b) unfolded bandstructure of 6-monolayer InAlAs on InP substrate.

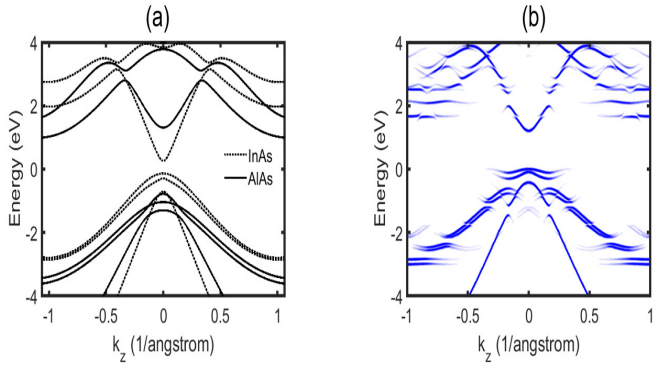

Fig. 2. Unfolded bandstructure of 6-monolayer InAlAs under (a) contraction- where substrate lattice constant is less than InP substrate and (b) expansion- where substrate lattice constant is greater than InP substrate.

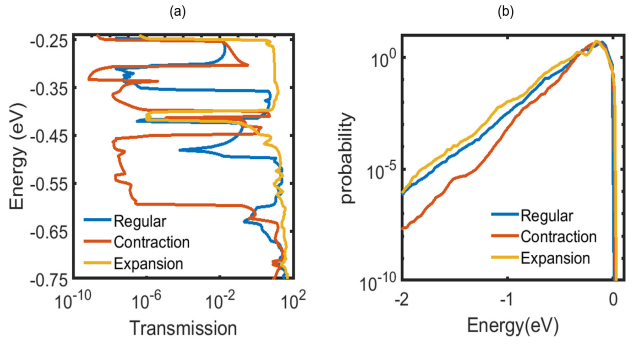

Fig. 4. (a) Ballistic Transmission vs. Energy plot in the valence band for regular, contraction and expansions cases computed using NEGF model under a bias of $0.25V$. (b) Carrier occupation probability vs. Energy in the valence band under electric field of $1MV/cm$.

III. Conclusion

In this work, we demonstrate that we can precisely compute the bandstructure of III-V digital alloy structures using the EDTB model which accurately incorporates the interface chemistry and an unfolding technique that can simply bandstructure of large structures. Furthermore, we utilize a NEGF model and Boltzmann transport solver to study the carrier transport in the digital alloys. These tools provide a great way to study and understand the electronic properties of different materials.

Acknowledgment

This work was funded by National Science Foundation grant NSF 1936016. The authors thank Dr. John P David of University of Sheffield and Dr. Seth R. Bank of University of Texas-Austin for important discussions and insights. The calculations are done using the computational resources from High-Performance Computing systems at the University of Virginia (Rivanna) and the Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by National Science Foundation grant number ACI-1548562.

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