Understanding the role of minigaps in APDs: Towards designing a better photodetector

Sheikh Z. Ahmed*, Jiyuan Zheng*, Yaohua Tan†, Joe C. Campbell*, and Avik W. Ghosh*
*Department of Electrical and Computer Engineering, University of Virginia, Charlottesville, VA, USA
†Synopsys, California, USA

***Abstract*—Superior performance of digital alloy APDs is attributed to the formation of "minigaps" in the material bandstructure. However, no improvement is observed in dilute nitride APDs in presence of minigaps. We propose criteria which can judge the effectiveness of these minigaps.**

I. Introduction

Avalanche photodiodes (APDs) are being increasingly used as ultra-sensitive receivers in a broad range of applications including communication, military and research applications. For operation in the short-wave infrared spectrum low noise and high gain-bandwidth product are the desired characteristics of a good APD. The internal gain resulting from carrier multiplication due to impact ionization culminates into the high sensitivity of these photodetectors. However, excess noise generated due to the stochastic nature of the impact ionization process limits the performance of these APDs[1]. The excess noise can be reduced by limiting the carrier multiplication origin to only one type of carrier, either electrons or holes. One way of doing this is introducing minigaps in the valence/conduction band and prevent carriers from reaching the ionization threshold energy. Minigaps have been observed in dilute nitride and digital alloys[2], [3]. However, improved performance is not observed in both of these APDs. In this paper we propose three inequalities that must be satisfied to see enhanced performance due to minigaps.

II. Band Structure

For our study, we use an environment dependent tight binding model, calibrated to Density Function Theory (DFT) bandstructures and wavefunctions, to calculate the bandstructure of III-V alloys[4]. In this model the interaction with the first nearest neighbour are incorporated into the calculations of the onsite energies and interatomic couplings of the tight binding hamiltonian to accurately capture the effect of strain. Using this model we compute the bandstructure of a supercell which yields a complicated bandstructure. To simply it, the bands of the supercell are mapped onto a primitive cell using a band unfolding technique. Fig. 1 shows the unfolded bandstructure of digital alloy InAlAs and AlInAsSb computed using this model. Minigaps are observed in the valence band (VB) of InAlAs and in the conduction band (CB) of AlInAsSb.

We believe that large bonding or onsite variations of frontier orbital result in these gaps. To illustrate this we built a simple

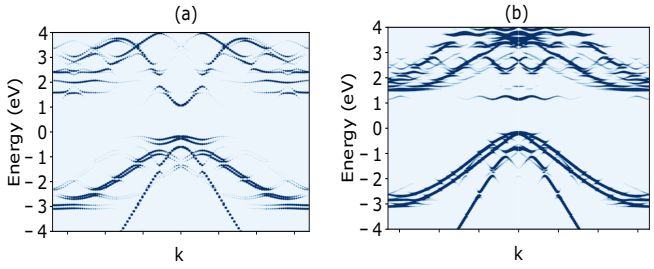

Fig. 1. Unfolded bandstructure of (a) 6-monolayer InAlAs and (b) AlInAsSb with 70% Al mole fraction.

1D toy model of a material chain consisting of two different arbitrary materials with varying VB offsets and zero CB offset. This is done by varying the hopping parameters between the materials. After applying our band unfolding technique we observe minigaps in the valence band, as shown in Fig. 2(a). Thus, as a first step, we need to identify the orbitals forming the concerned bands. This can be done by computing the orbital projected density of states (PDOS) from DFT calulations. Fig. 2(c) shows the PDOS of p_x orbitals of the InAlAs digital alloy. We observe here that it is mostly the p orbitals which are responsible for the bands near the valence band edge thus being the dominant orbitals responsible for minigaps. Further study of the onsite energies and interatomic couplings of these orbitals is imperative in creating a design rule for such APDs.

III. Inequalities

Based on bandstructure calculations and Monte Carlo simulations of these APDs we propose three inequalities that must be satisfied. These inequalities involving the band-width ΔE_b, miniband gap ΔE_G, ionization energy I, phonon frequency ω, electric field F and longitudinal effective mass m_l are:

$$\Delta E_b / I < 1 \tag{1}$$

$$\hbar\omega / \Delta E_G < 1 \tag{2}$$

$$exp\left(-\frac{4\sqrt{2m_l}\Delta E_G^{3/2}}{3q\hbar F}\right) << 1 \tag{3}$$

Firstly, to prevent ionization in the presence of these VB minigaps, it must be ensured that carriers do not reach the

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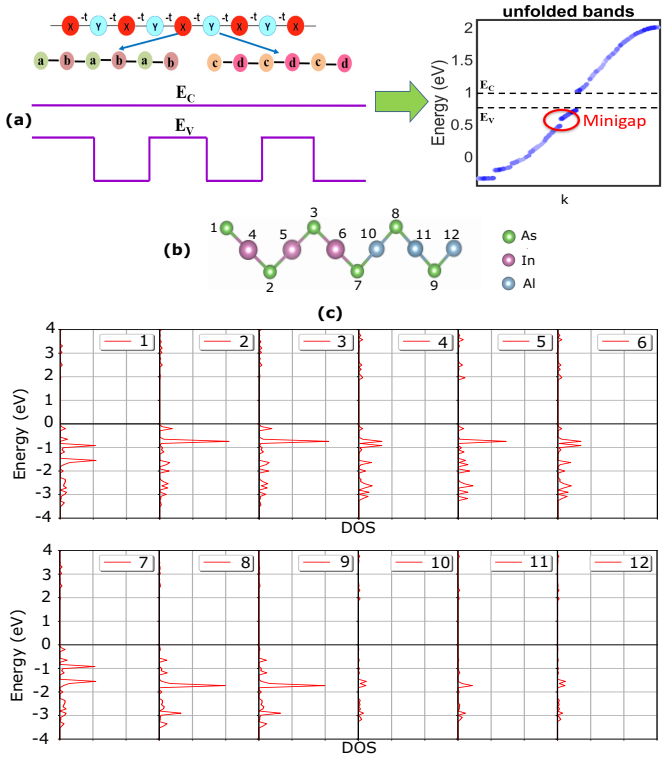

Fig. 2. (a) 1D toy model showing formation of minigaps by varying VB offsets. (b) supercell of InAlAs (c) Energy vs. projected density of states (PDOS) of p_x orbitals of InAlAs.

ionization threshold before reaching the minigap. This is reflected in the first inequality. The second one signifies that the minigap size needs to be greater than the optical phonon energy of the material in order to prevent carriers from reaching higher energy levels by optical phonon scattering. To prevent carriers from tunneling across the minigap the third inequality must be satisfied. This inequality is derived based on the famous Fowler-Nordheim equation used for computing tunneling probability at high electric fields across a triangular barrier[5].

TABLE I

Material	Inq. 1	Inq. 2	Inq. 3
InAlAs	0.20	0.45	0.15
InGaAs	0.59	0.85	0.67
AlGaAs	1.42	∞	1
AlInAsSb	0.26	0.28	0.04
GaAsN	0.20	0.36	0.46

Based on the inequalities above we can explain the performance discrepancy between the dilute nitride GaAsN APDs and III-V digital alloy APDs in the presence of minigaps. Table I lists the values of these inequalities for different materials used in APDs. Cells marked in green mean favorable for use in APDs and red marked ones being unfavorable. Minigaps are seen in the conduction band of GaAsN APDs and in the valence band of some digital alloy APDs. For both GaAsN

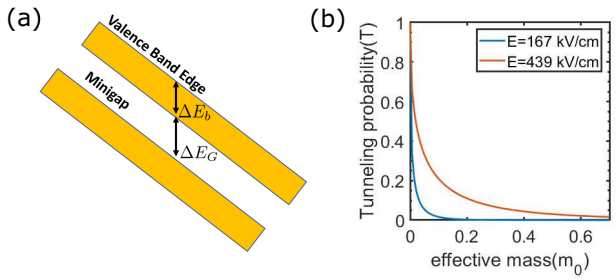

Fig. 3. (a) Band-width of first band and minigap in the valence band. (b) Tunneling probability vs. effective mass at different electric fields. Low effective results in a large increase in the tunneling probability which can enable electrons to tunnel across minigaps.

and InAlAs $\Delta E_G \approx 100\ meV$ which is significantly greater than the optical phonon energy and their band-widths are less than the ionization energy. However, the longitudinal effective masses of the sub-band near the minigap for the two materials are different. For GaAsN we consider $m_l = 0.025m_0$ and for InAlAs $m_l = 0.2m_0$. The tunneling probability, computed using the Fowler-Nordheim equation, for different effective masses are plotted in Fig. 3(b) for low and high electric fields. From the plot it is evident that as effective mass decrease the tunneling probability increases significantly. Thus, we can concur that electrons can tunnel across the minigap in GaAsN APDs and cause impact ionization. As a result, noise reduction is not observed in these dilute nitride APDs. This observation in effect also confirms the validity of the inequalities. Minigaps of about $400meV$ are also observed at the Γ point in the CB of AlInAsSb. Due to the large size of the gap the tunneling probability is very low. However, as the minigap size reduces away from the Γ point, we believe that the electrons can reach higher energies by means of inter-valley scattering and indirect band-to-band tunneling.

IV. Conclusion

In this work, we have established three criteria that when met can result in low excess noise in APDs in the presence of tiny gaps within the electronic bands. These gaps selectively limit the avalanche multiplication to a single carrier type. Based on these criteria we can engineer other materials suitable for high performance APDs that can be used for detection purposes of the other ranges of the electromagnetic spectrum.

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