

Full band Monte Carlo simulation of AlInAsSb digital alloys

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Abstract

Avalanche photodiodes fabricated from AlInAsSb grown as a digital alloy exhibit low excess noise. In this article, we investigate the band structure-related mechanisms that influence impact ionization. Band-structures calculated using an empirical tight-binding method and Monte Carlo simulations reveal that the mini-gaps in the conduction band do not inhibit electron impact ionization. Good agreement between the full band Monte Carlo simulations and measured noise characteristics is demonstrated.

KEYWORDS

AlInAsSb, avalanche photodiode, digital alloy, first principle study

1 | INTRODUCTION

For optical communications and data transmission applications, high-sensitivity receivers can reduce energy consumption and system cost. The internal gain of avalanche photodiodes (APDs) can provide a sensitivity advantage relative to p-i-n photodiodes. The excess noise factor of an APD, which arises from the random nature of impact ionization, is a key factor in the receiver sensitivity. The excess noise power density can be expressed as $\Phi = 2qIR(\omega)M^2F(M)$,¹ where q , I , and R represent electron charge, current, and device impedance, respectively. In the local-field model, $F(M) = kM + (1 - k)(1 - 1/M)$,

where k is the ratio of the hole ionization coefficient, β , to that of the electron, α .¹ The excess noise increases with gain but increases more slowly for low k values. The highest APD receiver sensitivities in the fiber optic 1310 and 1550 nm transmission windows have been achieved by InGaAs/InAlAs and Ge/Si separated absorption, charge, and multiplication (SACM) structures. The performance of InGaAs/InAlAs SACM APDs is limited by their relatively high k value, 0.2. While the k value of Ge/Si APDs is an order of magnitude lower, the large lattice mismatch between Ge and Si gives rise to large dark current, which yields noise comparable to InGaAs/InAlAs. Recently, an AlInAsSb digital alloy-based APD has been demonstrated to have low k (~ 0.01) and low dark current. In this paper, we use an empirical tight-binding method to calculate the band structure and Monte Carlo simulations to

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analyze the physical mechanisms responsible for low noise in this material system.

Random alloys of $\text{Al}_x\text{In}_{1-x}\text{As}_y\text{Sb}_{1-y}$ with a high Al content exhibit a wide miscibility gap. A recent set of experiments and calculations on APDs have uncovered some highly promising design possibilities hitherto unexplored in the field. This involves the ability by the Banks group at UT to grow certain digital alloys, such as $\text{Al}_x\text{In}_{1-x}\text{As}_y\text{Sb}_{1-y}$ with a high Al content, which in random alloys exhibit a wide miscibility gap.^{2,3} Recently, it has been reported that high-Al-content $\text{Al}_x\text{In}_{1-x}\text{As}_y\text{Sb}_{1-y}$ can be grown within the miscibility gap by MBE as a digital alloy of the component binaries, AlAs, AlSb, InAs, and InSb.⁴ In this work, we consider 70% Al composition. As shown in Figure 1A, each period consists of 3 monolayers (ML) InAs, 3 ML AlSb, 1 ML AlAs, and 3 ML AlSb. The 3D band-structure has been calculated using an empirical tight-binding model.⁵⁻⁷ The model is environmentally dependent, which means the strain and the interface issue have been considered in the calculation. The empirical parameter was adjusted iteratively to fit empirical tight-binding results with a hybrid functional band structure. In this work, we used the environment-dependent sp3d5s* tight binding-model introduced in Reference 5. The band-structure from the Γ point along the (001) direction is shown in Figure 1B. The bandgap is 1.19 eV. A large minigap is observed in the conduction band. Intuitively, a minigap in the conduction band would prevent electrons from achieving sufficient energy to impact ionize. However, previous work has shown that electron impact ionization occurs at a much higher rate than that of holes in the AlInAsSb digital alloy.⁸ In this article, full band structure based Monte Carlo simulation is used to analyze carrier transport.⁹⁻¹²

The first Brillouin zone is divided into 3D meshes ($19 \times 19 \times 19$); 46 conduction bands and 24 valence bands are included. Deformation scattering and impact

ionization are included in the Monte Carlo simulation. The carrier is considered to be in free flight between scattering events. The 3D based deformation scattering rate $P_{\nu\nu',\eta}^{\text{def}}(\mathbf{k}, \Omega_{\mathbf{k}\pm\mathbf{q}})$ from a point $\mathbf{k}$ in band ν to a region $\Omega_{\mathbf{k}'}$, in band ν' centered around $\mathbf{k}'$ can be derived from the Fermi Golden Rule and expressed as^{9,10}

$$P_{\nu\nu',\eta}^{\text{def}}(\mathbf{k}, \Omega_{\mathbf{k}\pm\mathbf{q}}) = \frac{\pi}{\rho\omega_{\eta\mathbf{q}}} |\Delta^\eta(\nu', \mathbf{k}, \mathbf{q}, \nu)|^2 |I(\nu, \nu'; \mathbf{k}, \mathbf{k} \pm \mathbf{q})|^2 D_{\nu'}(E', \Omega_{\mathbf{k}'}) \left(N_{\eta\mathbf{q}} + \frac{1}{2} \mp \frac{1}{2} \right) \quad (1)$$

where ρ is the lattice density, $\mathbf{q}$ is the phonon wave vector of mode η , and $\Delta^\eta(\nu', \mathbf{k}, \mathbf{q}, \nu)$ is the deformation potential, which is taken to be 0.73 eV/Å in the conduction band and 0.21 eV/Å in the valence band for this calculation.^{13,14} It should be noticed that the deformation potential value was taken from the value of InAlAs digital alloy as an approximation. $I(\nu, \nu'; \mathbf{k}, \mathbf{k} \pm \mathbf{q})$ is the overlap integral between the initial and final states, and $D_{\nu'}(E', \Omega_{\mathbf{k}'})$ is the density of states in $\Omega_{\mathbf{k}'}$, at energy $E' = E(k) \pm \hbar\omega_{\eta\mathbf{q}}$. $\hbar\omega_{\eta\mathbf{q}}$ is the phonon energy. Here, acoustic and optical phonon energies are taken to be the arithmetic average of the value for InSb (acoustic: 8 meV, optical: 25 meV) and AlAs (acoustic: 15 meV, optical: 50 meV).¹⁵ $N_{\eta\mathbf{q}} = \frac{1}{\exp(\hbar\omega_{\eta\mathbf{q}}/k_B T) - 1}$ denote the phonon occupation number. In this work, $T = 300$ K.

The Keldysh model is used to calculate the ionization rate and expressed as

$$P_{\nu\nu'}(\mathbf{k}, \mathbf{k}') = S(E - E_{th})^\gamma, \quad (2)$$

where E_{th} is the threshold energy, S is the softness parameter and γ is an approaching index. The Keldysh

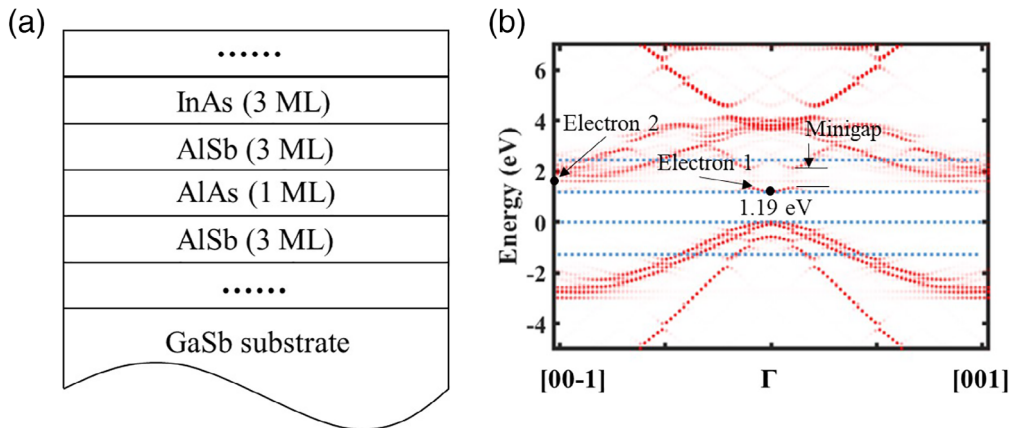


FIGURE 1 A, Lattice structures for AlInAsSb digital alloy and B, band structure and the two types of initial states of electrons in Monte Carlo simulation

parameters for electron and holes were adjusted by fitting the Gain curve and excess noise factor of Monte Carlo simulation results with experimental results. More detailed information about the Keldysh model (including how the parameters are fitted) can be found in References 16, 17. The parameters are provided in Table 1.

In experiment, the epitaxial structure of the digital alloy APD from top to bottom is 100 nm p-GaSb ($1 \times 10^{19} \text{ cm}^{-3}$), 100 nm p-Al_{0.7}InAsSb ($2 \times 10^{18} \text{ cm}^{-3}$), 1000 nm un-doped Al_{0.7}InAsSb, 200 nm n-Al_{0.7}InAsSb ($2 \times 10^{18} \text{ cm}^{-3}$). In the simulation, we take a simplification that the electric field distributes uniformly in the 1000 nm un-doped region and the depletion width is ignored. The simulated and measured gain curves are plotted in Figure 2A as dashed and solid curves, respectively. Figure 2B shows the simulated ($\blacktriangleleft$) and measured ($\blacktriangleright$) excess noise factor vs gain. The simulation results are consistent with experimental results.¹⁸

In our previous study, minigap in InAlAs digital alloy has been found to play an important role in influencing the ionization coefficient of holes.^{13,14,19} The accelerating path of holes is blocked by minigap and hole energy is not enough to trigger ionizations. Thereafter, an extremely low k value has been realized in InAlAs digital alloy. As shown in Figure 1B, a large minigap has been found in the conduction band of AlInAsSb digital alloy, while, there is no significant minigap in the valence band. If the minigap in conduction band could block electrons like the case in the valence band of InAlAs digital alloy, we can infer that the ionization coefficient of electrons is lower than that of holes. However, we found

TABLE 1 Electron and hole parameters in the Keldysh model

	S	E_{th}	γ
Electron	2.1×10^{14}	1.2	1
Hole	1.4×10^{15}	1.4	1.1

in the experiment that the electron ionization coefficient is much larger than holes.⁸ Apparently, minigap in the conduction band of AlInAsSb does not block the accelerating path of electrons, the electrons could find the path to jump across the minigap and gather enough energy to trigger ionizations. To verify this hypothesis, the transportation process of electrons is simulated based on full-band Monte Carlo simulation. Electrons that have an initial state above minigap and below minigap are analyzed and compared. As shown in Figure 1B, electrons 1 and 2 are located at the Γ point (below minigap) and the first Brillouin zone boundary along (00-1) direction (above minigap), respectively. Electron 1 starts from the lower energy state and has to surmount the minigap to achieve sufficient energy to trigger ionizations. Electron 2 starts from a state above minigap and does not have the same energy barrier. The propagations of both electrons are tracked and the energies are recorded every 1 fs. The sampling points are over 1 million. According to the law of large numbers, if the sampling data is large enough, the energy distribution of one electron (or hole) can reflect that of all electrons (or holes). The energy distribution probability (normalized to the total number of

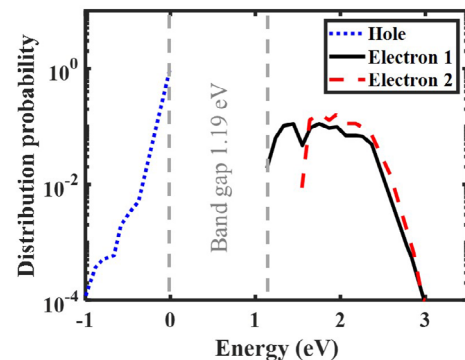


FIGURE 3 Energy distributions for carriers in AlInAsSb, wherein electrons with two types of initial states are compared

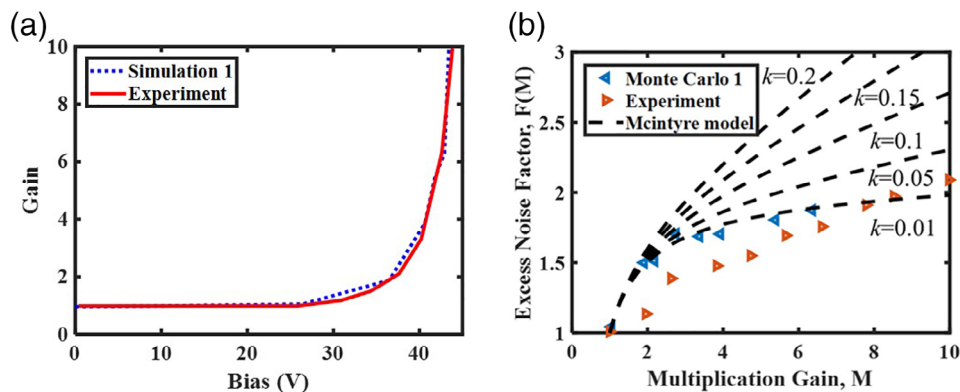


FIGURE 2 Full band-based Monte Carlo simulations for A, gain vs bias B, excess noise factor vs gain, M

TABLE 2 Effective masses for simplified single parabolic bandstructure

	Γ (001)	L (111)	X (100)	HH (001)	LH (001)	SO (001)
Effective mass (m_0)	0.06	1.9	0.1	0.4	0.38	0.08

TABLE 3 Important energy parameter

	Bandgap	Split-off band energy gap	Energy step to the first mini-gap in the valence band	First minigap in valence band	Acoustic phonon energy	Optical phonon energy
Energy (eV)	1.19	0.48	0.66	0.2	0.0165	0.0364

sampling points) for the two types of electrons under an electric field of 439 kV/cm are shown in Figure 3. The electric field is taken considering the total bias is 43.9 V (avalanche gain is 10), avalanche region thickness is 1 μm and the electric field is uniformly distributed. There is little difference in the high-energy portion of the energy distributions, which indicates that the minigap does not prevent electrons from accumulating the energy required to impact ionize.

As was explained in our previous work,¹³ although the energy is discontinuous in the (001) direction, there are in-plane energy states that have sufficient energy to go across the minigap. The electrons that are scattered to these in-plane states can get over the minigap under the driving force of the electric field. In the simulation, the energy of electron 2 did not drop below the minigap because the 439 kV/cm electric field is high enough to enable electrons to accelerate to higher energy states. In addition, there are fewer energy states in the minigap energy level for electrons to relax to. The energies of holes are also shown in Figure 3. It can be seen that holes tend to occupy low energy states. The hole energies are smaller than the bandgap and do not trigger ionizations. It follows that the ionization coefficient of holes is much smaller than that of electrons.

In this work, 3D band structure is used to deploy Monte Carlo simulation. To have an intuitive physical analysis of the energy distribution of carriers, some band structure parameters along different crystal directions are calculated and put in Table 2. Important energy parameters are provided in Table 3.

Given the disparity between the electron mass and that of the hole in the heavy hole and light hole bands, it can be concluded that the split-off (SO) band plays a critical role in hole acceleration. Large separation (0.48 eV) between the heavy-light hole bands and the SO band impedes impact ionization. The energy step to the first mini-gap is 0.66 eV, which is much smaller than bandgap (1.19 eV). Since the first mini-gap has an energy of 0.2 eV, which is much larger than phonon energy, the holes could not jump across the minigap by the help of phonon scatterings. Since the hole energy distribution is

much more limited than that of the electron, we can infer that it is not easy for holes to find a path (in 3D Brillouin zone) to get over minigap like electrons.

2 | CONCLUSION

In this paper, we present calculations of the band structure of digital alloy AlInAsSb. APDs fabricated from AlInAsSb exhibit the lowest noise of any III-V compound material. By analyzing the band structure calculated by the empirical tight-binding method, we have shown that there are minigaps in both the conduction band and valence band. Full band structure based Monte Carlo simulation shows that minigap in the conduction band does not block the electron accelerating process. The hole accelerating process is limited, wherein large effective mass and minigap might play an important role. Good agreement between the full band Monte Carlo simulations and measured noise characteristics is demonstrated.

CONFLICT OF INTEREST

The authors declare no conflict of interest.

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