Theoretical D* Optimization of N+-p Pb1−xSnxSe Long-Wavelength (8 - 11 µm) Photovoltaic Detector at 77 K

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ABSTRACT

In this work, the study of the influences of lifetime, doping concentration and absorption layer thickness to resistant-area product (R0A) and quantum efficiency of Pb1−xSnxSe photovoltaic detector are presented. Three fundamental current mechanisms including diffusion, generation-recombination, and tunneling models are considered. Using optimal doping concentration and absorption layer thickness parameters, the calculated detectivity (D*) of Pb1−xSnxSe photovoltaic detector is over 1012 cm Hz1/2/W.

KEYWORDS

Pb1−xSnxSe; Lifetime; Resistant-Area Product; Quantum Efficiency; Detectivity

1. Introduction

Mid- and long-infrared light detection in the atmosphere windows (3 - 5 um and 8 - 14 um) has widespread military and civilian applications. There is an increasing demand to have a large format and long wave infrared imaging system. Existing technologies are mainly based on semiconductor photo-detectors [1]. HgCdTe (MCT) is currently the premier material of interest for mid- and long-wave IR focal plane array (FPA) applications. The best MCT material is produced by MBE on CdZnTe substrates. However, these substrates are costly, brittle, and of small size. For large format FPA applications, many major players are transferring the growth and processes of MCT to alternative substrates, mainly Silicon. The transfer is complicated by a 19% lattice mismatch and nearly 100% thermal mismatch. The results are a mid- to high- 10^6 cm^-2 dislocation density which has deleterious effect on the final FPA. Other alternatives such as III-V materials are facing similar challenges pertaining to the large-sized substrate.

IV-VI semiconductors such as Pb1−xSnxSe offer high sensitivity similar to MCT [2]. Until the end of the 1970s, both materials were intensively developed with comparable effort for mid-IR detector applications. MCT became predominantly the material of choice mainly because the permittivity of IV-VI materials is lower than that of MCT, which leads to slow RC response time. At that time, the concerns pertaining to the single-element detector were legitimate. However, this argument does not apply to staring imaging systems that contain a large number of sensors. The large dielectric constant, which is more than 10 times that of MCT, becomes advantageous because coulomb scattering by ionized impurities is strongly suppressed. Consequently, the electric field caused by such defects is shielded within a very short distance. Therefore, IV-VI Pb-salt materials are much more tolerant to defects in comparison to MCT. Due to this effect, Pb-salt materials could have approximately one order of magnitude higher performance than MCT for the same dislocation density [3].

It has been demonstrated that high quality IV-VI semiconductors can be grown on Si substrate. The mismatch of the thermal expansion coefficient was well addressed by a thin CaF2 buffer layer. Dislocation gliding on (111)-
oriented substrate reduces the threading dislocation density caused by lattice and thermal expansion mismatch [4]. Recently, we have developed a growth method for IV-IV materials on Si substrate that reduces the etch pit density down to $10^5$ cm$^{-2}$ [5]. These advantages make IV-VI materials promising candidates for large-format long wave infrared FPA [6].

In this paper, we present a theoretical investigation for IV-VI Pb$_{1-x}$Sn$_x$Se in the long wavelength spectral range (8 - 11 $\mu$m). The influences of different generation-recombination mechanisms to the carrier lifetime are discussed. The resistant-area product ($R_oA$) is divided into three parts for the discussion: diffusion, recombination in junction area, and tunneling. The optimized doping concentration and layer thickness are calculated. The optimized detectivity is over $10^{12}$ cm Hz$^{1/2}$/W.

2. Theory

2.1. Carrier Lifetime

The carrier generation-recombination mechanisms in detector devices are distinguished as band to band Auger’s, radiative and Shockley-Read-Hall’s (SRH) generation-recombination mechanisms. Among them, SRH’s mechanism is determined by the material quality. Auger’s and radiative mechanisms are determined by energy band structures. Therefore, those two are fundamentally limiting factors for the overall generation-recombination processes. In this paper, we consider only Auger’s and radiative mechanisms to examine the PbSnSe material system. More realistic simulation can be performed by considering SRH’s mechanism for a given material quality. For the radiative process, in case of the Boltzmann statistics, the carrier lifetime is determined by [7]:

$$\tau_r^{-1} = 2B\left(\frac{N_i^2}{4} + n_i^2\right)^{1/2},$$

where

$$B = \frac{2n_i q^2 (2p_i^2 + p_i^2) E_g^4}{9\pi^2 h^4 c^3 (p_i^3 n_i^3)^2 F(\beta)}.$$

$N_i$ is the acceptor concentration which is assumed to be equal to the major carrier concentration in $p$-type layer, and $n_i$ is the intrinsic carrier concentration. The function $F(\beta)$ is defined as:

$$F(\beta) = \frac{1}{\beta^{1/2}} \int_0^{\infty} \sqrt{1 + \frac{r^2}{\beta}} \left(3 + 8t/\beta + 8t^2/\beta^2\right) \times \exp(-\beta - 2t) dt$$

in which $\beta = E_g/(k_BT)$, $n_i$ is the refractive index, $p_i$ and $p_i$ are the momentum matrix elements, $E_g$ is the band gap energy. Based on the experimental data, it is reasonable to assume that the doping concentration $N_i \gg n_i$, consequently, the corresponding carrier lifetime leads to

$$\tau_r = 1/(N_i B).$$

For the carrier lifetime depending on Auger’s process, the relationship is given by

$$\tau_a^{-1} = \left[C_a (N_i^2 + 2n_i^2)^{1/4}\right]^{-1}$$

[8]. In the case of $N_i \gg n_i$, the simplified Auger’s carrier lifetime equation is derived as

$$\tau_a^{-1} = \left(C_a N_i^{2}\right)^{-1}.$$  

The Auger’s recombination coefficient $C_a$ is defined as [9]:

$$C_a = \frac{3q^4 (2\pi)^{5/2} (k_BT)^{1/2} E_g^{-7/2} h^3}{(16\pi e_0 e_o)^{7/2} m_i^{11/2} m_i^{3/2}} \times \exp\left[-\frac{E_g}{2k_BT}\left(\frac{m_i^*}{m_i}\right)^{-1}\right],$$

where $m_i^*$ and $m_i^*$ are the longitudinal and transverse effective masses.

2.2. Resistant Area Product ($R_oA$)

For the $R_oA$ calculation, we made following assumptions in our model. Firstly, the photodiode in this model is $N^+ - p$ hetero-structure (the capital letter means the material has larger band gap energy, symbol “+” denotes high doping concentration). The lightly doped $p$-type layer is sandwiched between the substrate silicon and highly doped, wider band gap $N^+$ layer. The wider band gap $N^+$ layer has smaller absorbance and lower intrinsic carrier concentration. In such a structure, the $p$-type absorption layer determines both dark current $I_D$ and photocurrent $I_p$ of the diode. Secondly, the carrier lifetime is only determined by Auger and radiative mechanisms. Thirdly, we assume the carrier mobility at 77 K is a constant value of $2 \times 10^6$ cm$^2$/V$s$. Fourthly, the dark current is determined by diffusion-drift, generation-recombination and tunneling mechanisms. Finally, we assume that the front side surface is well passivated. Due to the backside illumination mode (light incident through substrate side) and the wider-gap layer, influence of surface recombination on the top surface can be eliminated. The schematic band diagram of epitaxial $N^+ - p$ Pb$_{1-x}$Sn$_x$Se hetero-junction photodiode is presented in Figure 1.

The $R_oA$ product is contributed by diffusion-drift ($R_oA_{DD}$), generation-recombination ($R_oA_{GR}$) and tunneling ($R_oA_T$) processes:

$$(R_oA)^{-1} = (R_oA_{DD})^{-1} + (R_oA_{GR})^{-1} + (R_oA_T)^{-1}.$$ 

The $R_oA_T$ product derived from diffusion current is given by

$$R_oA_{DD} = \frac{k_BT L_n}{q^2 D_n n_p} \coth\left(\frac{w_p}{L_n}\right)$$ [10],

where $D_n$ is the diffusion coefficient, $L_n$ is the electron diffusion length which is equal to $\sqrt{D_n \tau_n}$, $w_p$ is the thickness of $p$ layer, $n_p$ is the minority concentration in $p$ layer. The generation-recombination $R_oA_{GR}$ determined by the depletion area current is expressed by the equation

$$R_oA_{GR} \text{,}$$

with $\text{Detection}$
are the orientation dependent
is the absorption coefficient
( )
and
is the photon flux at the edge of the absorption layer 
Valley shown as follows [14]:

ciency. Its formula is slightly modified in this work and used to increase transmission close to unity. In this work, the substrate Si. However, antireflection coating can be used to increase transmission close to unity. In this work, we assume the light incidence is 100% transmission.

In the hetero-junction structure, Rosenfeld etc. used the tunneling mechanism is given by

where \( m_i \), \( m_i^* \), and \( m_i^* \) are the orientation dependent effective mass components. For IV-VI materials, they are given in Table 1.

2.3. Quantum Efficiency

The reflectivity of radiation is a limiting factor for quantum efficiency. IV-VI group materials have very large dielectric constants. As a result, for the frontside illumination mode, the reflection loss can be more than 50%, for the backside illumination mode, the loss just decreases down to 30% due to the lower dielectric constant of the substrate Si. However, antireflection coating can be used to increase transmission close to unity. In this work, we assume the light incidence is 100% transmission.

In the hetero-junction structure, Rosenfeld etc. used one dimensional model to derive the net quantum efficiency. Its formula is slightly modified in this work and shown as follows [14]:

where

\[
G_{l,z} = \left[ \frac{2 \pi m_i^* \epsilon_0}{q m_i^* \epsilon_0^* \frac{E_g}{E_g^2}} \right]^{1/2} \exp \left( \frac{q^2 \sqrt{2 N_s m_i^* m_i^* / m_i^*}}{2 \hbar N_d} \right) [12],
\]

where the monochromatic backside illumination generation rate \( G_l(z) \) is defined as

\[
G_L = \alpha(z) \varphi_0 \exp \left[ -\int_0^z \alpha(u) du \right],
\]

in which \( \varphi_0 \) is the photon flux at the edge of the absorption layer (\( z = 0 \)) and \( \alpha(z) \) is the absorption coefficient which is dependent on Sn composition. It is given by the two band model relation

\[
\alpha = \frac{\sqrt{2}}{5} \frac{q^2 m_i \left( 2 m_i^2 + m_i^* \right)}{\pi n c \epsilon_0 \hbar^2 E_g} \times \left[ \frac{2 \left( \hbar \omega \right)^2 + E_g\hbar^2}{3 \left( \hbar \omega \right)^2} \right]^{1/2},
\]

in which \( \omega \) stands for the angle frequency of the incident light.

The quantum efficiency described above is associated with the monochromatic photon flux. However, the detectors are normally exposed to a wide spectral range flux as described by Plank’s radiation law. Consequently, the weighted average of the quantum efficiency can be given by

\[
\eta_{AVE} = \frac{\int_{\lambda_{min}}^{\lambda_{max}} \eta(\lambda) n(\lambda) d\lambda}{\int_{\lambda_{min}}^{\lambda_{max}} n(\lambda) d\lambda},
\]

where \( n(\lambda) \) is the spectral radiant photon emittance of the target.

2.4. Detectivity

The detectivity is the most important figure of merit for detectors. The Johnson-Nyquist noise dependent detec-

Table 1. Orientation dependent effective mass [13].

<table>
<thead>
<tr>
<th>Orientation</th>
<th>( m_i )</th>
<th>( m_i^* )</th>
<th>( m_i^* )</th>
<th>Valley</th>
</tr>
</thead>
<tbody>
<tr>
<td>[111]</td>
<td>( m_i )</td>
<td>( m_i^* )</td>
<td>( m_i^* )</td>
<td>( m_i^* )</td>
</tr>
<tr>
<td>[110]</td>
<td>( 2m_i + m_i^* )</td>
<td>( 2m_i + m_i^* )</td>
<td>( 3m_i + m_i^* )</td>
<td>( m_i^* )</td>
</tr>
<tr>
<td>[100]</td>
<td>( 2m_i + m_i^* )</td>
<td>( 2m_i + m_i^* )</td>
<td>( 3m_i + m_i^* )</td>
<td>( m_i^* )</td>
</tr>
</tbody>
</table>

where \( m_i \), \( m_i^* \), and \( m_i^* \) are the orientation dependent effective mass components. For IV-VI materials, they are given in Table 1.
tivity is given by \( D^* = \frac{q\eta\lambda}{4\hbar k T} \). From this formula, it is denoted that \( D^* \) is associated with both resistant area product \( R_0A \) and quantum efficiency \( \eta \). Shot noise dependent detectivity is not discussed in our model.

3. Results and Discussions

3.1. Optimization of Doping Concentration

The parameters for the simulation are listed in Table 2. As can be seen, all of the parameters except mobility and \( \varepsilon_\infty \) are dependent on Sn composition and the temperature. In terms of this condition, the simulated results should be convincible in \( \text{Pb}_{1-x}\text{Sn}_x\text{Se} \) system. The Sn compositions of 0.053 and 0 are used for p-type \( \text{Pb}_{0.947}\text{Sn}_{0.053}\text{Se} \) layer and \( \text{N}^+\text{PbSe} \) layer, respectively.

Figure 2 shows Auger’s lifetime (solid dot), radiative lifetime (solid square) and the total lifetime (solid line) with acceptor concentration in p layer of \( \text{Pb}_{0.947}\text{Sn}_{0.053}\text{Se} \). While \( N_A \) is larger than \( 1 \times 10^{17} \text{ cm}^{-3} \), Auger’s mechanism dominates the material lifetime. The lifetime is less than 10 ns when the doping concentration is \( 2 \times 10^{17} \text{ cm}^{-3} \). When \( N_A \) is lower than \( 1 \times 10^{17} \text{ cm}^{-3} \), lifetime influenced by the radiative mechanism is increasing more slowly than the Auger’s one. The lifetime is over 100 ns when concentration is \( 3 \times 10^{16} \text{ cm}^{-3} \). This is because Auger’s lifetime is proportional to \( N_A^{-2} \) and radiative lifetime is proportional to \( N_A^{-1} \). In all, total lifetime decreases rapidly with the increase of \( N_A \).

Figure 3 shows the \( R_0A \) for different doping concentrations \( N_d \) at 77 K. The thickness of \( p \) layer is 16 \( \mu \text{m} \). Three mechanisms are taken into consideration. The resistant area product \( R_0A \) caused by the tunneling process is proportional to exponential \( N_d^{-1} \), as a result, \( R_0A \) drops dramatically as \( N_d \) is over \( 1 \times 10^{17} \text{ cm}^{-3} \). Overall, \( R_0A \) decreases with the increase of \( N_d \), and the value varies slightly when \( N_d \) is under \( 1 \times 10^{17} \text{ cm}^{-3} \).

Therefore, both lifetime and \( R_0A \) increase as the acceptor concentration \( N_d \) decreases. Since the typical \( N_d \) for \( \text{Pn}_{1-x}\text{Sn}_x\text{Se} \) is between \( 1 \times 10^{16} \text{ cm}^{-3} \) and \( 1 \times 10^{17} \text{ cm}^{-3} \) at 77 K, we use \( N_d \) of \( 3 \times 10^{16} \text{ cm}^{-3} \). The corresponding lifetime is approximately 100 ns. The diffusion length \( L_n \) is 36.4 \( \mu \text{m} \). In this case, the diffusion length is twice as long as the absorption thickness. Thus, all carriers generated in this layer will be collected.

3.2. Optimization of the Thickness of Absorption Layer

The quantum efficiency is sensitive to the thickness of the absorption layer. Based on the discussion above, we use a lifetime of 100 ns and \( N_d \) of \( 3 \times 10^{16} \text{ cm}^{-3} \), and the energy band gap of 0.115 eV. (Corresponding wavelength is 11 \( \mu \text{m} \).) Figure 4 shows the relationship between

Table 2. Physics properties of \( \text{Pb}_{1-x}\text{Sn}_x\text{Se} \) [11], [16], [17].

<table>
<thead>
<tr>
<th>Parameters</th>
<th>( \text{Pb}_{1-x}\text{Sn}_x\text{Se} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E_g(x,T) )</td>
<td>( 0.125 - 1.021 x + (4 \times 10^{-7} + 2.56 \times 10^{-7} \times T^2) )</td>
</tr>
<tr>
<td>( m_e^* )</td>
<td>( [20.7 \times E_g(0,0)/E_g(x,T) + 4.3]\times m_e )</td>
</tr>
<tr>
<td>( m_h^* )</td>
<td>( [11.4 \times E_g(0,0)/E_g(x,T) + 2.9]\times m_h )</td>
</tr>
<tr>
<td>( m_e^* )</td>
<td>( [20.7 \times E_g(0,0)/E_g(x,T) + 8.7]\times m_e )</td>
</tr>
<tr>
<td>( m_h^* )</td>
<td>( [11.4 \times E_g(0,0)/E_g(x,T) + 3.3]\times m_h )</td>
</tr>
<tr>
<td>( \varepsilon_\infty )</td>
<td>( (107/E_g)^{0.66} )</td>
</tr>
<tr>
<td>( n_e )</td>
<td>( (107/E_g)^{0.66} )</td>
</tr>
<tr>
<td>( \varepsilon_\infty )</td>
<td>227 at 77 K</td>
</tr>
<tr>
<td>( \mu_s )</td>
<td>( 2 \times 10^4 \text{ cm}^2/\text{Vs} )</td>
</tr>
</tbody>
</table>

Figure 2. Lifetime versus acceptor concentrations at 77 K.

Figure 3. The resistant area product \( R_0A \) versus acceptor concentration \( N_d \) at 77 K.
quantum efficiency and absorption thickness in the long wavelength spectral range 8 to 11 μm. In this figure, quantum efficiencies decrease as incident wavelength increases. As can been seen, 12 μm thickness gives the highest value of about 95% at 8 μm.

We apply weighted average of quantum efficiency to define the optimal thickness with the best performance. The background radiation temperature is at 300 K. The simulation result is given in Figure 5. It denotes average quantum efficiency rising rapidly from 8 μm to 14 μm. And around 16 μm thickness, the quantum efficiency value reaches the peak.

3.3. Detectivity

With the calculated quantum efficiency and lifetime value. Figure 6 shows the simulated $D^*$ for different Pb$_{1-x}$Sn$_x$Se p-type layer thickness at 77 K. For thickness between 10 to 18 μm, $D^*$ value is over $10^{12}$ cm Hz$^{1/2}$/W.

To our knowledge, the highest reported theoretical $D^*$ for HgCdTe N+-p photodiode in long wavelength spectral range (8 - 11 μm) is $9 \times 10^{10}$ cm Hz$^{1/2}$/W at 77 K [18]. We would like to point out that their simulation included the surface recombination process with a surface recombination velocity (SRV) of $10^4$ cm/s. When we consider surface recombination using the same SRV the $R_0A$ changed slightly from 41 to 40 ohm·cm$^2$. Since quantum efficiency depends weakly on SRV our simulated $D^*$ value remains almost the same. This $D^*$ value of Pb$_{1-x}$Sn$_x$Se is more than one order of magnitude larger than the simulated $D^*$ of MCT’s in reference [18].

4. Conclusion

The one dimensional Pb$_{1-x}$Sn$_x$Se photovoltaic diode simulation model has been discussed in this work. We calculated the lifetime, $R_0A$, absorption, quantum efficiency and detectivity for structure N+-p heterojunction on Si substrate. The optimized $D^*$ value obtained is over $10^{12}$ cm Hz$^{1/2}$/W. This result indicates a great potential for PbSnSe detector with superior detectivity to be fabricated.

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REFERENCES


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Dislocations and Ionized Impurities in PbSe and MCT,”


