The Numerical–Experimental Enhanced Analysis of HOT MCT Barrier Infrared Detectors

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We present the results of numerical simulations and experimental data of band gap-engineered higher operating temperature mercury cadmium telluride barrier photodiodes working in a middle wavelength infrared radiation and a long wavelength infrared radiation range of an infrared radiation spectrum. Detailed numerical calculations of the detector performance were made with our own computer software taking into account Shockley Hall Read, Auger, band-to-band and trap-assisted tunneling and dislocation-related currents. We have also simulated a fluctuation phenomena by using our Langevin-like numerical method to analyze shot, diffusion, generation–recombination and $1/f$ noise.

Key words: HOT MCT barrier detectors, valence band offset, MOCVD technology

INTRODUCTION

Barrier mercury cadmium telluride (MCT) detectors arose as an attempt to reduce dark current in high-temperature infrared detectors generated at contacts, space charge and surface regions.^{1–8} Dark current caused by Shockley Hall Read (SHR) generation–recombination (G–R) processes associated with metal vacancies and dislocations is a very important issue. These SHR mechanisms are intensified by a trap-assisted tunneling (TAT) process. Blocking the passage of the electron current by a barrier in the conduction band effectively reduces dark current and increases dynamic resistance of the detector. Moreover, the existence of a wide band-gap barrier suppresses SHR dark current. Another positive development is the suppression of Auger^{9–12} and surface currents.

A non-zero valence band offset in MCT-based barrier detector structures is the key item limiting

their performance,^{6–8,13–15} because holes generated by an optical absorption are not able to overcome the valence band energy barrier. Relatively high bias is required to be applied to collect photo-generated carriers. However, this might lead to a strong band-to-band (BTB) and TAT due to a high electric field within the depletion layer. Grading of the barrier helps reduce the valence band-offset and increase the offset in a conduction band when appropriately combined with a proper p -type doping.^{13–17}

In this work, we present numerical simulations and experimental results for a long and middle wavelength of infrared spectrum (LWIR and MWIR) MCT barrier detectors. The calculations take into account a wide spectrum of G–R processes containing Auger 1 and Auger 7, as well as SHR mechanisms dependent on the concentration of trap centers associated with the metal vacancies and misfit dislocations generated in the process of MOCVD growth. We neglected the radiative recombination due to a strong reabsorption effect in MCT. In Ref. 18, we conducted an extensive discussion of

the impact of different mechanisms of G–R on $j(V)$ characteristics in barrier detectors. A detailed description of parameters for SHR, Auger 1 and Auger 7 lifetimes is included in Ref. 18 and references cited here. Carrier mobility is calculated theoretically as it was presented in Ref. 19. It seems to us that readers will be familiar with this problem by reading the mentioned article. Calculations were carried out by using an original computer software elaborated by K. Jóźwikowski and A. Jóźwikowska.

We have also analyzed for some years^{19–21} fluctuation phenomena by using our Langevin-like numerical method developed by Jóźwikowski, and now it enables the determining of the noise current spectrum in heterostructures. In addition, we also determined distributions of noise power density caused by fluctuations of Joule power. This enables the determining of different noise sources and areas where the noise power is mainly generated. This is useful for devices' optimal design. Photoelectrical parameters numerically determined were compared with the performance of the manufactured detectors.

NUMERICAL SIMULATIONS

Objects

We have considered two MESA barrier detectors working in an MWIR and LWIR wavelength range shown in Fig. 1. Spatial distributions of mole fraction, donor, and acceptor concentrations are shown along the axis of symmetry of the structures (shown in Fig. 1) are presented in Fig. 2. All the spatial distributions of physical parameters shown in next figures of the devices apply to the line being the symmetry axis. An absorber of about $3\ \mu\text{m}$ thickness was applied in an LWIR structure in order to increase the response speed and suppress the Auger generation at lower voltages.

Methods

The analysis of the structures was carried out by solving the set of transport equations. The details can be found in our previous work (see, e.g., Refs. 20–22). Similarly as in Ref. 21, we have determined Auger 1 and Auger 7 as well as SHR generation rates caused by metal vacancies and dislocations. BTB and TAT were also included. The vacancy concentration assumed at the level of $10^{14}\ \text{cm}^{-3}$ in all volume of two considered devices gives the best fit to the experimental results. In the calculations, we assume a $10^6\ \text{cm}^{-2}$ dislocation density in whole structures except for areas where the density of dislocations is increased (Fig. 7a and b) according to the Yoshikawa relationship.²³ Details about assumed activation energies and cross-sections of traps caused by vacancies and dislocations are the same as in Refs. 21 and 22.

We set inter-band absorption coefficients using the Anderson's relationships²⁴ taking into account

Fig. 1. Architecture of the half cross-section of cylindrical barrier mesa structures, (a) MWIR detector, (b) LWIR detector.

the Burstein–Moss effect. The absorption Urbach tail was also included.²⁵ A single reflection from the upper contact was assumed

The key to modeling fluctuation phenomena in semiconductors is a solution of a set of transport equations for fluctuations (TEFF), derived by Jóźwikowski,¹⁹ modified and developed in subsequent works, Refs. 20, 21, and 26.

TEFF becomes the set of Langevin-like equations if we can determine the random source terms i.e.

Fig. 2. Spatial distribution of CdTe mole fraction x , donor concentration N_D , and acceptor concentration N_A for structures presented in Fig. 1. (a) MWIR structure, (b) LWIR structure.

$\delta\tau_{\text{rel}}^e$, $\delta\tau_{\text{rel}}^h$, $\delta(G-R)_{\text{SHOT}}$, $\delta(G-R)_{1/f}$, $F_C(t)$, $G_C(t)$, $F_n(t)$ and $F_p(t)$. Here $\delta\tau_{\text{rel}}^e$, $\delta\tau_{\text{rel}}^h$ are the fluctuations of electron relaxation time and hole relaxation time, respectively. Kousik et al.,²⁷ based on Handel's theory of $1/f$ noise,^{28,29} obtained theoretically spectral intensity of $\delta\tau_{\text{rel}}^e$ for silicon. We have adopted their results for HgCdTe in some previous works.^{19–21,26} Handel's theory of $1/f$ noise is based on the fact that, in accordance with the quantum electromagnetic field theory, electric charge carriers are accompanied by photons. Interactions leading to the change in carrier velocity are sources of creation or annihilation of photons (Bremsstrahlung). They are called “soft photons” and are not energetic enough to be detected; however, the possibility of their absorption or emission must be taken into account in the calculation of scattering amplitude. The number of these photons is inversely proportional to their energy. This way, both scattering processes determined by relaxation time and G–R processes determined by G–R terms are the potential sources of $1/f$ noise. In our previous paper, Ref. 21, we have determined the Hooge coefficients³⁰ for $1/f$ noise caused by Auger 1, Auger 7, radiative and SHR G–R mechanisms. The influence of dislocations

on $1/f$ noise was also determined. These noise sources are included in TEFF in $\delta(G-R)_{1/f}$ terms. $F_C(t)$ denotes the fluctuation of a heat stream and $G_C(t)$ denotes the fluctuation of a heat generation rate.²⁶ $F_n(t)$ and $F_p(t)$ denote electron and hole diffusion noise, respectively.^{31,32} In the presented structures, diffusion noise plays a marginal role and these two sources may be omitted. Similarly to Ref. 21, the dislocations' influence on noise current was also taken into account in this paper. By solving TEFF, we can determine the spatial distribution of the temperature fluctuations, electrical potential fluctuations and quasi-Fermi energies fluctuations for electron and holes for an arbitrarily chosen frequency in a $\Delta f = 1$ Hz frequency range. On their basis, we can calculate the fluctuation of all physical quantities contained in the set of transport equations. The effect of the noise generation within the device is the noise current observed at the electronic circuit connected with the element. The connection between the current noise observed in the electronic circuit and the fluctuations of current density inside the detector were described in Ref. 21. Results of our calculations presented in our earlier paper were verified with experimental results of other researchers. The problem of $1/f$ noise in HgCdTe photodiodes was analyzed by many researchers. Usually, two current models of $1/f$ noise are considered in the literature: for example, the McWhorter model³³ developed by Anderson and Hoffman,³⁴ Hsu,³⁵ Schiebel,³⁶ and Kinch et al.,³⁷ and Hooge's model³⁰ developed, for example, in Ref. 27. McWhorter model treats free carrier density fluctuations as the noise source, but Hooge's model assumes fluctuations in the mobility of free charge carriers to be the noise generation mechanisms. However, in our opinion, these two models can be easily combined by using the Handel' theory.

NUMERICAL AND EXPERIMENTAL RESULTS

Figure 3a shows measured and calculated normalized current–voltage $j(V)$ characteristics for an MWIR detector. A slight increase in the current in the reverse direction for a bias voltage above 0.2 V is caused mainly by TAT in the space charge region on the border between absorber area and N^+ region. This phenomenon is strongly dependent upon the concentration of metals' vacancies and dislocation density.³⁸ To determine the tunneling probability, the WKB method is used,³⁹ and we approximate the shape of a potential barrier. In our software, we can use three possibilities: triangular, parabolic and hyperbolic barriers. Calculations presented in Fig. 3a were carried out for the hyperbolic barrier (thin solid lines) and for the triangular barrier (bold solid lines). One can find slight differences in the characteristics of the theoretical waveforms $j(V)$. Characteristics are drawn in a logarithmic scale and the TAT effect is poorly visible. If we used a linear

Fig. 3. Calculated (solid lines) and experimental (dashed lines) normalized current–voltage $j(V)$ characteristics; (a) MWIR detector, (b) LWIR detector.

scale, the TAT effect would be much more evident. At present, we are developing the model of TAT phenomenon in MCT structures where the shape approximation of a potential barrier is more realistic.

Figure 3b shows $j(V)$ characteristics for an LWIR barrier detector, typical for Auger-suppressed devices with a significant internal resistance. Reverse bias initially increases dark current and gradually depletes the absorber in minority and majority carriers. A significant part of the applied voltage drops across internal series resistance. At sufficiently large bias, the suppression of Auger generation starts to reduce dark current which also reduces voltage drop across the series resistance, causing more bias on the heterostructure and rapid drop of dark current. Calculations are carried out assuming the normalized series resistance equal to $0.05\ \Omega$ and trap density $N_T = 10^{14}\text{cm}^{-3}$ and $N_T = 10^{15}\text{cm}^{-3}$.

The band structures of the devices are presented in Fig. 4. The effective carrier lifetime is also affected by the supply voltage (Fig. 5). The reason for this is a depletion in carrier concentration. A

Fig. 4. Calculated band diagram for MOCVD grown MCT detectors; (a) MWIR detector, (b) LWIR detector.

strong decrease in minority carrier concentration in the absorber region is observed after biasing in a reverse direction in both structures. In the LWIR detector, the concentration of majority holes is also strongly decreased (Fig. 6), which leads to a strong decrease in Auger 7 generation rate and increase in carrier lifetime in LWIR devices. The influence of the bias voltage on the carrier lifetime at room temperature is presented in Fig. 5a and b. In the LWIR device in the whole area of absorber, one can observe the strong increase in carrier lifetime with the increase in bias voltage in a reverse direction up to 500 mV . Further increasing the voltage does not change the carrier lifetime. In the MWIR device, biasing practically does not change the carrier lifetime in the absorber region except for the interface between the absorber and the N^+ layer. But the increase of bias voltage in MWIR devices leads to a decrease in carrier lifetime due to the increase of SHR generation caused by TAT in a strong electric field. In MWIR structures, there is a decisive impact of SHR thermal generation in the N^+ -p space charge region. Moreover, with the increase in the reverse bias voltage, the SHR generation is increased due to TAT.¹⁸ Exclusion, however, has a very strong influence on the thermal generation in LWIR structures. This is due to the fact that the thermal generation is mainly caused by

Fig. 5. Calculated spatial distribution of carrier lifetime; (a) MWIR detector, (b) LWIR detector.

Auger mechanisms in the absorber area. In the MWIR detector, the highest SHR generation is located at the interface of the N^+ –absorber. The slight increase of thermal generation in this place after biasing structures in a reverse direction (Fig. 7a) is caused by TAT. Electrons generated by the strong thermal generation in a cap contact layer in the LWIR structure (Fig. 7b) are effectively blocked by the barrier.

Figure 8a shows the current responsivity of the MWIR detector in 300 K and 260 K biased with 600 mV in reverse a direction. Solid lines show the experimental results, and points show the results of calculations at 300 K. We observed a weak dependence on the supply voltage in the range of -0.1 V to -1 V. Maximum responsivity is observed for a wavelength equal to about $3 \mu\text{m}$ and is equal to about 1 A/W. The calculated values are almost two times higher, but in calculations of radiation reflectance, the influence of series and preamplifier resistance were not taken into account.

Figure 8b shows the current responsivity of the LWIR detector in 300 K for different supply voltages as a function of light wavelength. Maximum

Fig. 6. Calculated spatial distribution of the electron (n) and holes (p) concentration for MOCVD grown MCT detectors; (a) MWIR detector, (b) LWIR detector.

responsivity is observed for a wavelength equal to about $5.5 \mu\text{m}$. In the absence of the bias voltage the sensitivity is below 0.1 A/W. The biasing in a reverse direction increases the responsivity to >2 A/W for the voltage of -0.3 V. However, for the bias voltage equal to -1 V, it is about 1 A/W. Reducing the current responsivity with increasing voltage can be explained by the influence of series resistance and the influence of the suppression of Auger generation. An optical generation starts to increase the current, which also increases voltage drop across the series resistance causing less bias on the heterostructure and reducing the suppression of Auger generation.

Figure 9a shows the spectral density of noise current in the MWIR detector. When the detector is biased in a reverse direction, the G–R noise dominates for frequencies above several dozens of Hz. For smaller frequencies, $1/f$ noise dominates, induced mainly by fluctuations of mobility.^{19–21} Forward bias significantly increases the noise current. Similar conclusions can be drawn by analyzing Fig. 9b for the LWIR detector. In this case, $1/f$ noise dominates for frequencies below 1 MHz. The calculations were carried out for mesa detectors with a surface area equal to $18,100 \mu\text{m}^2$. The assumed trap concentration is equal to 10^{14} cm^{-3} in both detectors. Biasing the LWIR detector in a reverse

Fig. 7. Spatial distribution of dislocation density (dashed line) and thermal generation rate; (a) MWIR detector, (b) LWIR detector.

direction leads to a decrease in noise current. This is caused by a decrease of carrier concentration due to the extraction and exclusion effect in the absorber region and in N^+p interface. Decrease of carrier concentration also appears when the semiconductor structure is cooled and cooling reduces fluctuations of the Joule heat treated in our method as a fluctuation of noise power. The noise power density is mainly generated in an N^+p interface region both in the MWIR and LWIR detector (see Fig. 10a, b, and c). Further testing would require the appropriate choice of gradient composition and doping of interface to reduce the noise generation in the area.

Figure 10 show the spatial distribution of spectral density of noise power density in MWIR and LWIR structures. Figure 10a and b show the distribution at 300 K in detectors biased with -1 V for 1 Hz and 1 MHz of frequency. Figure 9c shows this distribution for 1 MHz of frequency in the LWIR structure when the detector is biased with -1 V and -0.1 V . One can notice a decrease of noise power density with an increase of bias voltage.

The tested devices were fabricated in a joint laboratory MUT and VIGO System S.A. The (111) HgCdTe layers were grown on 2-in. (c.50-mm), epitaxially, semi-insulating (100) GaAs substrates,

Fig. 8. Current responsivity as a function of wavelength for an LWIR detector. Solid lines show the experimental results. Points show the results of calculations; (a) MWIR detector, (b) LWIR detector.

oriented 2° off toward the nearest $\langle 110 \rangle$. Typically, a 3- to 4- μm -thick CdTe layer was used as a buffer layer reducing stress caused by a crystal lattice misfit between a GaAs substrate and a HgCdTe epitaxial layer structure.⁴⁰ The growth was carried out at a temperature of 350°C and mercury zone at 210°C using the interdiffused multilayer process (IMP)^{41,42} in a horizontal MOCVD AIX 200 reactor. Hydrogen was used as a carrier gas. The reactor pressure of 500 mbar was used for all successful growth runs. Dimethylcadmium (DMCd) and diisopropyltelluride (DIPTe) were used as precursors of Cd and Te. The n - and p -type doping was achieved by in situ doping with iodine and arsenic, respectively. Ethyl iodine (EI) was used as a donor and TDMAAs as an acceptor of dopant sources. The II/VI mole ratio was kept in the range from 1.5 to 5 during CdTe cycles of the IMP process. The temperature of mercury was controlled by an external heater that also maintained control of the reactor cell ceiling temperature profile. The growth was completed with a cooling procedure at metal-rich ambient. The obtained heterostructures were not annealed ex situ, however.⁴³ MOCVD technology

Fig. 9. Calculated spectral density of noise current as a function of frequency for chosen bias voltage; (a) MWIR detector, (b) LWIR detector.

with a wide range of composition and acceptor/donor doping and without post-grown annealing is an excellent tool for HgCdTe heterostructures' epitaxial growth. More comprehensive details of the growth are presented in Refs. 2, 4, and 43.

CONCLUSIONS

The properties of higher operating temperature (HOT) HgCdTe barrier detectors operating in the MWIR and LWIR range of infrared spectrum were simulated and confronted with experimental data for MOCVD-grown heterostructural photodiodes. The following conclusions can be drawn from the studies:

- The valence band offset can be minimized with a proper selection of composition and p -type doping profiles.
- The dark current and high frequency noise in both in the MWIR and LWIR barrier devices is mainly generated by the Auger 1 and Auger 7 inter-band mechanisms, additionally enhanced by the SHR processes related to metal vacancies and dislocations.

Fig. 10. Spatial distribution of spectral noise power density. (a) MWIR detector, (b) LWIR detector, (c) LWIR structure at 300K for 1MHz of frequency.

- Noise current is generated mainly at the interface between the absorber and the N^+ electron contact. The low-frequency noise is caused by fluctuations of electron and hole mobility.
- The noise could be reduced with a refinement of the devices' architecture by a proper selection of the composition and doping level grading especially in an N^+ -absorber interface. It needs additional theoretical and experimental investigations.

ACKNOWLEDGEMENTS

The work has been done under the financial support of the Polish National Science Centre as research Projects 2013/08/A/ST5/00773, 2013/08/M/ST7/00913 and PBS 653.

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