CdZnTe Radiation Detectors with HgTe/HgCdTe Superlattice

Contacts for Leakage Current Reduction

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ABSTRACT

CdZnTe-based heterojunction $p-i-n$ or $M-\pi-n$ detectors using HgTe/CdTe superlattice contacts are modeled and designed to reduce leakage currents under high electric fields and thereby improve X-ray and γ -ray detector performance. The employment of an n-type HgTe/CdTe superlattice as a contact layer can theoretically result in significantly less leakage current compared to a contact layer using either bulk semiconductors or metal contacts. The benefits arise from the ability to design HgTe/CdTe superlattices to have large carrier effective masses in the electric field direction, which results in low carrier velocities. Nevertheless the density of states is lower than that of a comparable bulk semiconductor, which results in low carrier concentrations.

Keywords: superlattice, cadmium zinc telluride, radiation detector, leakage current

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1. INTRODUCTION

Advanced radiation detectors with high energy resolution, linear energy response and the capability of room temperature operation for both normal counting and spectroscopic mode operation are highly desirable for numerous applications such as medical diagnosis, astrophysical exploration, non-destructive industrial evaluations, homeland security and counterterrorism inspections as well as nuclear proliferation detection to ensure national and international nuclear safety. State-of-the-art, room temperature, high resolution X-ray and γ -ray detectors are usually based on CdZnTe semiconductors. The current standard device configuration for CdZnTe-based detectors employs high quality, high resistance CdZnTe material to form photoconductive or homojunction devices with two metal contacts ($M\pi M$ configuration), which are either Ohmic or non-Ohmic. Some recent device designs for single carrier species collection, including coplanar¹⁻⁴ and Frisch-grid⁵⁻⁷/Frisch-ring⁸⁻¹⁰ detectors, use a similar geometry. Low leakage currents are especially desirable since they directly correlate with noise performance, which is very important for applications at low photon flux or high temperatures. In particular, reducing leakage current is also equally important for astrophysical hard X-ray applications where such devices are also used and continue to be improved. In addition, a large leakage current also corresponds to high energy dissipation, which turns out to be a bottleneck in the utilization of large scale array detectors. An increase in the band gap with a larger Zn composition in CdZnTe is beneficial in the reduction of leakage currents; however, this is accompanied by a reduction in the absorption coefficient and hence the efficiency. Such a trade-off confines the Zn composition to the range of 10 to 20% depending on the energy of the hard X-ray or γ -ray photons and cannot be increased appreciably. The current state-of-the-art technique is based on the balance of compensated impurities, which must be carefully established during either bulk growth or after

growth thermal treatment procedures. Although great progress has been made in the improvement of material quality, restrictions in state-of-the-art bulk growth techniques still exist, and in particular their yields are low. Some of these issues are associated with the purification of precursors or bulk material growth, and some of these may be due to the non-stoichiometric nature of CdZnTe. Because these issues will continue to exist in the foreseeable future, other approaches for improvements must be explored. Optimizing the device architecture design is also very effective in leakage current suppression. Schottky barriers between metal contacts and semiconductors have been introduced to form Schottky junctions and hence to reduce charge carrier injection. Although these structures possess relatively good properties, the low surface barrier results in relatively high leakage currents under moderate bias.¹¹ In addition, the leakage mechanism is still determined by majority carriers. A semiconductor $p-n$ junction has also been employed to reduce leakage currents since the leakage current in a $p-n$ junction is determined by the minority carrier. Further suppression of leakage currents at higher electrical fields can be achieved using a $p-i-n$ device that yields much better detector performance,^{12, 13}. This is particularly valuable for high energy γ -ray detection with high resolution due to its capability to offer a much broader depletion region and a more uniform electrical field in the device. Advantages of a $p-i-n$ structure can also be obtained by changing to a $M-\pi-n$ structure, i.e. replacing the p contact with a low metal-semiconductor barrier to form a quasi-Ohmic contact.¹¹ Operational $p-i-n$ CdTe detectors have been reproducibly fabricated with the aid of epitaxial HgCdTe contact layers. Heterojunction $p-i-n$ HgCdTe/CdZnTe/HgCdTe detectors were made by growing n - or p -type HgCdTe on opposite faces of a bulk CdZnTe substrate using liquid phase epitaxy (LPE) techniques, as reported by Hamilton and co-workers.^{14, 15} The energy resolution of 1.82% FWHM for ^{133}Ba 0.356 MeV was achieved, using a bulk CdZnTe substrate material

with a nominal 4% Zn composition, which matches the HgCdTe lattice constant. These experimental or prototype devices confirmed that the heterojunction $p-i-n$ device configuration is well-suited for suppressing leakage currents and enhancing detector performance.

In this paper, we report a model, design, and an alternative approach to the fabrication of CdZnTe-based heterojunction $p-i-n$ detectors whose primary goal is to reduce leakage currents, permit increased bias voltages and therefore improve their performance, particularly at hard X-ray and γ -ray wavelengths. In this approach, a HgTe/HgCdTe superlattice (SL) is grown on a pretreated, passivated and polished CdTe or CdZnTe bulk substrate via molecular beam epitaxy (MBE). We show below that this proposed structure is theoretically superior to HgCdTe/CdZnTe/HgCdTe $p-i-n$ detectors. The benefits arise because the SLs can be designed to have large carrier effective masses along the electric field direction¹⁶ that will strongly inhibit leakage currents, yet a density of states less than that of a comparable bulk semiconductor. Moreover, the HgTe and HgCdTe thicknesses can be so chosen such that the resulting SL is approximately lattice matched to the CdZnTe substrate, thereby ensuring excellent crystalline quality. In addition to the expected reduction in leakage currents, it has been demonstrated that such SLs prevent the propagation of dislocations present in the underlying crystal and smooth out surface roughness¹⁷, both of which are beneficial for the formation of uniform electrical fields and increased detector resolution.

2. ELECTRONIC ENERGY BAND STRUCTURE CALCULATIONS OF RELATED SEMICONDUCTOR MATERIALS AND STRUCTURES

Device modeling and design were conducted based on sets of material and device parameters. All these parameters are not readily available from experimental sources, hence theoretical electronic band structure calculations were conducted to obtain key parameters that

are required for device simulations. The parameters of interest include the energy band gap, carrier effective masses and the density of states. Our calculations of the electronic band structure of the semiconductor materials and structures such as CdZnTe, HgCdTe and HgTe/CdTe SLs are based on the either 8 or 14 bulk basis band k·p method. The use a 14-band basis rather than the more common 8-band basis arises because of the sensitivity of the optical and electronic properties to the electronic structure in the deeper secondary regions of the band structure. Errors inherent in the 8-band model become significantly more pronounced when the states of interest are far from the center of the Brillouin zone. Spin-orbit splitting is included in these calculations.

HgTe/CdTe SLs possess a Type III band alignment and have many unique properties. HgTe is a semimetal due to its inverted band gap. When SLs are formed by alternatively growing thin layers of HgTe and HgCdTe, the electronic energy band structure perpendicular to the growth direction, namely along the x direction, will exhibit zone folding. At low temperatures, when the HgTe well thicknesses is less than c.a. 6 nm, the SL possess a normal CdTe-like semiconductor band structure, shown in Fig.1, whereas when the HgTe well is larger than c.a. 6 nm, shown in Fig.1, the SL possess an inverted HgTe-like band structure. By adjusting the thickness of both the HgTe well and HgCdTe barrier, one can design a SL with an energy band gap from 0 to that of CdTe. The reason for considering $\text{Hg}_{0.05}\text{Cd}_{0.95}\text{Te}$ rather than CdTe barriers is that a Hg flux must be provided during MBE growth to maintained high crystal quality. Specifically, 5% Hg is typically incorporated into CdTe barriers if the growth is performed on a (211)B surface, while roughly 30% Hg is incorporated if growth is performed on a (100) surface. The calculations reported here assume a (211)B surface. No significant difference in Hg composition is expected if growth takes place on a (111) surface rather than (211)B since the

latter is tilted by only 19.4° from the (111) plane along the $[\bar{1}11]$ direction.

We are currently employing both 8-band (with spherical or cubic symmetry) and 14-band $k \cdot p$ (cubic symmetry) second principles models to calculate the SL electronic band structures and optical absorption coefficients, which have been compared with experimental optical absorption data. The input parameters need to be finely tuned based on experimental results.

The device architecture used in our model is a metal, compensated semiconductor, and n-type semiconductor, namely $aM-\pi-n$ configuration (with the π region being CdZnTe and the n region being a HgTe/Hg_{0.05}Cd_{0.95}Te SL). The anode of the detector is a HgTe/Hg_{0.05}Cd_{0.95}Te SL together with a metal contact, in which the SL is n-type doped to various carrier concentrations from 10^{15} to 10^{20} cm^{-3} . The device is modeled under a reverse bias of 1 kV/cm. To suppress leakage currents while maintaining high detector performance, the SL involved in the n-type contact prototype device should have a large hole effective mass along the electrical field direction, to minimize the hole velocity along the field direction, while its density of states in the valence band (N_v) should be small, to minimize the number of holes. This requirement can be fulfilled if we design our SL to possess a large effective mass along the growth direction while reducing the effective masses perpendicular to the growth direction relative to bulk HgCdTe. The calculated electron and hole effective mass as functions of HgTe well and HgCdTe barrier thicknesses are shown in Fig.2.

3. DEVICE MODELING AND DESIGN

This section discusses two comparisons: $aM-\pi-n$ device with a SL as the n-type layer vs. a traditional $M-\pi-M$ one, and a $M-\pi-n$ device with a SL as the n-type layer vs. a $M-\pi-n$ device with a HgCdTe alloy as the n-type layer.

1) $M-\pi-n$ device with a SL as the n-type layer vs. a traditional $M-\pi-M$ one

To our knowledge, no commercially-available device simulation software package is capable of fully handling the tunneling and thermionic properties of highly anisotropic SL materials. We estimated the one-dimensional leakage current using a pseudo-SL material, whose material properties are largely the same as the HgCdTe alloy with the same band gap. Although the SLs are expected to have longer Auger recombination lifetimes than the alloy with the same band gap, our transport calculations assumed that the SL has the same recombination lifetimes as the alloy. This assumption will overestimate the ideal SL leakage current. We estimated the mobility of the carriers, including both electrons and holes, in pseudo-SL material using the electron mobility of a HgCdTe alloy (μ_e , calculated with the empirical formula suggested by Charlton and co-workers.¹⁸⁾ with the same band gap adjusted by the ratio of effective masses, namely the pseudo-SL mobility is $\mu_i = \mu_e \cdot m_e / m_i$, where m_e is electron effective mass of alloy, calculated by the formulas given by Wiley and Dexter¹⁹ and m_i is the pseudo-SL effective mass in the growth direction. The principal effects of SL transport are captured by the use of SL rather than bulk alloy effective masses in these calculations.

The leakage current of a *p-i-n* or *M- π -n* detector employing pseudo-SL n-type contacts can be calculated numerically using standard continuity and Poisson's equations together with some assumed boundary conditions. In this work, we employed the SimWindows software package (developed by Dr. David W. Winston, University of Colorado) for one-dimensional device transport simulations. Similar results were also obtained using other software packages, including AMPS-1D (developed by Stephen J. Fonash and co-workers, The Pennsylvania State University) and SCAPS (by Marc Burgelman, University of Gent, Belgium). Based on these material parameters, we calculated the leakage current of a CdZnTe detector with a *M- π -n* device architecture. The contact between the cathode metal and CdZnTe can be either Ohmic or

Schottky with a barrier up to 1.05 eV, which has a negligible impact on the leakage current under high biases, greater than 1 kV/cm. We used a pseudo-SL for the n-type layer. The anode metal contact to the SL was assumed Ohmic with negligible contact resistance. As an example, Fig.3 shows a reduction in leakage current from 10^{-5} Acm^{-2} without a pseudo-SL n-type layer (namely a direct metal contact to the CdZnTe) to several orders of magnitude lower in the SL case, with the doping level of the n-type SL determining the actual leakage current. We conclude that one can significantly reduce leakage currents in $M\text{-}\pi\text{-}M$ structures by replacing them with $M\text{-}\pi\text{-}n$ ones with the use of narrow band gap, pseudo-SL n-type layers with suitable doping levels. Such improvements arises because hole transport is impeded in a suitably designed narrow band gap pseudo-SL without a significant reduction in transport of majority electrons, which carry the signal. Increasing the SL doping level and band engineering the band-edge valence band density of states to a low value will reduce the minority carrier (hole) concentration, and consequently also reduces the leakage current. By increasing the doping level of the n-type SL, the leakage current of the detector can be suppressed by at least one order of magnitude relative to a standard $M\text{-}\pi\text{-}M$ device.

2) *M- π -n device with a SL as the n-type layer vs. a M- π -n device with a HgCdTe alloy as the n-type layer*

A more detailed analysis can be analytically performed to compare a $M\text{-}\pi\text{-}n$ device with a SL as the n-type layer with a $M\text{-}\pi\text{-}n$ device with a HgCdTe alloy as the n-type layer. After Perlman and Feucht²⁰, the current density through a heterojunction (here we consider the $\pi\text{-}n$ junction) under bias along the z direction can be written as

$$J_z = -\frac{q}{(2\pi)^3} \int d^3k f_1(U)[1 - f_2(U)]W(U_{z1}, U_{z2}, m_{z1}, m_{z2}) \frac{1}{\hbar} \frac{\partial U}{\partial k_{z1}}, \text{ which involves a 3-dimenional momentum}$$

(k) space integration over carrier distribution functions f_i ($i=1, 2$, corresponding to region 1, where carriers originate, and region 2, where carriers transport to) and transport probability function W . The carrier distribution functions f_1 and f_2 are functions of energy U in the corresponding device regions (U_i , $i=1$ in region 1 and $i=2$ in region 2). W is a function of the kinetic energy of the carriers along the current direction z in regions 1 (U_{z1}) and 2 (U_{z2}), as well as the effective masses along the current direction in regions 1 (m_{z1}) and 2 (m_{z2}). Since f and W are functions of energy, a Jacobean can be introduced in order to transfer from energy space to k space, for example as given by Searles and Pulfrey.²¹ In addition, q is the electron charge and $\hbar$ is the reduced Planck constant in the current expression. If we ignore the change in barrier height due to change of carrier effective mass from one region to another, which only dominates at very low temperatures²², we can rewrite the leakage current formula in the form of a general current $J_z \sim qvnW$, where n is carrier concentration, v is the carrier velocity, which for thermionic cases is the Richardson velocity $v_R = (k_B T / 2\pi m)^{1/2}$, and k_B is Boltzmann's constant. The transport probability W is equal to 1 for the thermionic case. In the case of tunneling, it can be estimated using the WKB approximation $W(U) \sim \exp[-\frac{2}{\hbar} \Delta z \sqrt{2m(V_0 - U)}]$, where V_0 is the barrier height at point z . Integration may be required based on the shape of barrier. Under a triangle barrier approximation, we can estimate W using the Fowler-Nordheim formula.²³ Since tunneling occurs in the CdZnTe region, W is independent of the properties of the SL or alloy n-type regions. We computed the leakage current ratio between diodes that use SL n-type contacts ($J_{z,SL}$) and alloy contacts $J_{z,Alloy}$ as $\frac{J_{z,SL}}{J_{z,Alloy}} = \sqrt{\frac{m_{z,Alloy}}{m_{z,SL}}} \cdot \frac{n_{SL}}{n_{Alloy}} = \sqrt{\frac{m_{z,Alloy}}{m_{z,SL}}} \frac{n_{i,SL}^2}{n_{i,Alloy}^2}$, where n_{SL} and n_{Alloy} are the densities of minority carriers that cross the junction and hence contribute to leakage currents. $n_{i,SL}$ and

$n_{i,Alloy}$ are the intrinsic carrier concentrations of the SL and alloy, respectively. $n_{i,SL}$ was calculated using the density of state effective mass that averages effective masses along the directions parallel and perpendicular to the current. $n_{i,Alloy}$ is obtained using the formula given by Hansen and co-workers.²⁴ We calculated the one-dimensional leakage current ratio J_{SL} / J_{Alloy} when using a SL or a HgCdTe alloy contact, both with the same band gap. We examined SLs with $Hg_{0.05}Cd_{0.95}Te$ barrier thicknesses up to 10.5 nm and HgTe well thicknesses up to 6 nm. Thicker HgTe wells will create inverted SL band structures that dramatically reduce Auger recombination lifetimes, therefore are not considered here. The calculated results of J_{SL} / J_{Alloy} are shown in Fig.4, which shows a decrease of J_{SL} / J_{Alloy} ratio decreasing energy gap. However, on the another hand, larger energy band gap materials have lower intrinsic carrier concentrations; such gaps favor leakage current reductions. Considering many assumptions have to be added into the calculation and modeling, modeling itself only results in a tendency of in J_{SL} / J_{Alloy} ratios vs. the variation of SL structural parameters. Modeling can also predict a promising exploration range of SL structures located near the employed 2nm HgTe well and 2nm HgCdTe barrier thicknesses, as shown in Fig.4(b). If the parameters are chosen properly, one can anticipate at least one order of magnitude leakage current reduction by employing $M-\pi-n$ device architecture involving pseudo-SL (as shown in Fig.3) plus another one order of magnitude leakage reduction by optimizing the SL as shown in Fig.4. Fine tuning of designed parameters has to be conducted and benchmarked based on test devices and experimental data.

4. CONCLUSIONS

The goal of our theoretical calculations and simulations was to optimize the design

parameters of CdZnTe absorber-based heterojunction $M-\pi-n$ detectors with SL contacts in order to achieve the best detector performance in terms of not only minimizing the leakage currents but also maintaining both high energy resolution and detection efficiency. We found that a HgTe/HgCdTe SL with the structure of about 2 nm HgTe well and 2 nm HgCdTe barrier thicknesses is the most promising design to realize low leakage currents. Such a design is anticipated to effectively reduce leakage currents by at least two orders of magnitude relative to detectors using the same CdZnTe absorbers but with only Ohmic metal contacts. In future work, the validity of the predictions is to be put to a test by fabricating the proposed device and measuring the leakage current and energy resolution as well.

ACKNOWLEDGEMENTS

This work was supported by Department of Energy, NNSA Service Center, Office of Nonproliferation Research and Development (NA-22) Proliferation Detection Program under grant number DE-FG52-08NA28765. We are also grateful to Prof. M.E. Flatte of the University of Iowa for permitting us using his 14 band k.p electronic band structure codes. We acknowledge the use of SimWindows software package that was developed by Dr. David W. Winston at the University of Colorado.

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FIGURE CAPTION

Fig.1: Computed band structures for HgTe/Hg_{0.05}Cd_{0.95}Te SLs with various HgTe well thickness

d_{HgTe} .

Fig.2: Computed room temperature carrier effective masses in HgTe/HgCdTe SLs as functions of well and barrier thicknesses. (a) Hole effective masses along the growth direction; (b) hole effective masses perpendicular to the growth direction; (c) electron effective masses along growth direction; and (d) electron effective masses perpendicular to the growth direction.

Fig.3: Room temperature leakage current density as a function of donor doping level of the n-type region (anode) in a $M-\pi-n$ radiation detector with the n-type region being a pseudo-SL, and under a bias of 1 kV/cm (red thick lines) or 2 kV/cm (blue thin lines). The dashed and dash-dot lines are for $M-\pi-M$ detectors with the π CdZnTe (CZT) absorber having $1 \times 10^8 \Omega \cdot cm$ resistivity and being under the same bias. (a) Pseudo-SL band gap at 360 meV, and (b) band gap at 200 meV. The inset of (a) is a band profile of the $M-\pi-n$ device under 2 kV/cm reverse bias, which show an energy barrier for hole injection into the CdZnTe. Electron flow from the CdZnTe into the n-type region is not impeded.

Fig.4: (a) White lines are calculated leakage current density ratios (SL to HgCdTe alloy)

expressed in percentage form as a function of HgTe well and HgCdTe barrier thickness.

Yellow lines show the band gap in meV as a function of well and barrier thicknesses. The rough region in the lower right corner corresponds to inverted band SL structures that are not considered in this project due to their extremely low carrier recombination lifetimes.

(b) A magnification of (a) near the 2 nm HgTe/2 nm Hg_{0.05}Cd_{0.95}Te region, with dashed lines giving the energy gap and solid lines the calculated leakage current density ratios (SL to HgCdTe alloy) expressed as percentages.