Chapter 5

A Schottky Diode Detector for the Terahertz Regime

5.1 Introduction

In the previous chapters, structures based on the n-i-p photodetectors having CdTe as a window have been discussed. This chapter reports the performance of a Schottky diode detector for the absorption wavelength of 30 µm. Graphene has been a promising candidate among 2 D materials that have greater photodetection applications [137]-[143]. It has become a prominent material in the development of photodetectors in the THz region [144]-[146]. Most of the photodetectors reported have been based on a bilayer or a multi-layer graphene (as semiconducting material) p-n and p-i-n structures which are responsible for the absorption of the incident radiation [147]-[149]. Since graphene is extremely thin, in pure form, it has the potential to be used as a semi-transparent material and the bandgap opened graphene as a semiconductor as well as a semi-transparent material. In a few Field Effect Transistors that were reported, graphene material has been used as the channel. Of late, graphene photodetectors were mainly used in the UV and visible regions [150]-[154]. Recent studies recommend that graphene in a single layer or few layers can be used for infrared and far infrared i.e., terahertz detection purposes [155]-[160]. In this chapter, a detailed analysis of optoelectronic characteristics of the Schottky diode detector operating at 30 µm wavelength i.e., at 10 THz frequency has been presented. The device analysis has been carried out in the commercially available numerical simulator ATLAS.

5.2 Structure Description

We have seen in the previous chapters that n-i-p photodetector structures (single heterojunction and double heterojunction) employed CdTe material as a window. Recently, You *et al.*, [159] reported that graphene forms a good adhesive contact with MCT and can be used for photodetection purposes. They have used hybrid graphene embedded in MCT for mid-IR wavelength applications. Also, conventionally the speed of the Schottky diodes has always been high. In general, if the contact is close to the active layer, the device will have less chance of recombination at the surface. This results in more radiation reaching the active layer thereby improvement in optical characteristics. Based on the above, we proposed a device comprising graphene as a metal contact and MCT as an active or absorbing material in the Schottky diode detector structure. Graphene is a semi-metal and is so thin that it is almost semi-transparent to the incoming THz radiation. Graphene has a work function of 4.56 eV [161] and it forms a Schottky contact with n-type MCT that has a work function of 4.25 eV. Hence, a Schottky diode is developed. MCT is grown epitaxially on the lattice-matched CdZnTe substrate. Graphene is transferred onto the MCT layer. It is assumed that the THz radiation is incident on the metal contact i.e., on graphene. As it is atomically very thin and has an absorption of only 2.3% [162]-[166], it allows most of the incoming THz radiation to reach the active layer (MCT). As the MCT-based devices suffer from large leakage currents at room temperature, the device has been operated at liquid nitrogen temperature. Since metal (graphene) can be directly deposited on the semiconductor (MCT) unlike the p-n diodes or p-i-n diodes where fabrication steps are more, fabrication cost gets reduced. It is a majority carrier device unlike a p-n or p-i-n diode where the dark current is mostly influenced by two minority carrier concentrations. This is the main reason for a low dark current in the Schottky diode. Therefore, reverse recovery time is less and we can use it as a switch. Here, we can use it as an optically controlled switch.

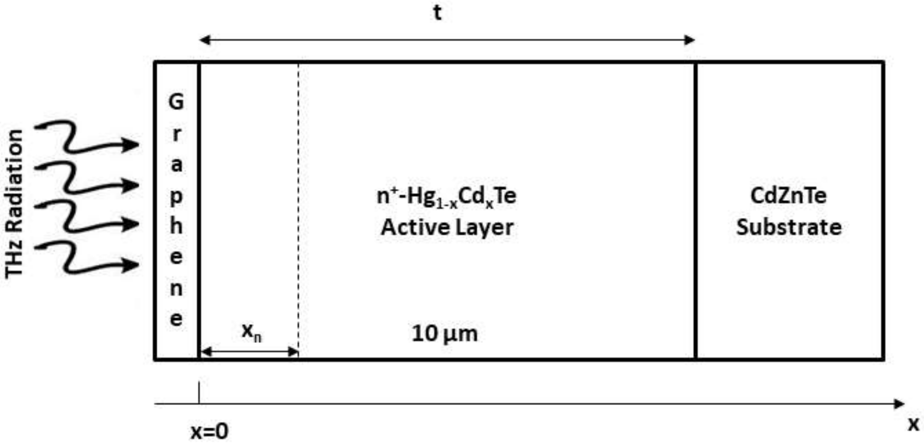

Fig.5.1 Schematic of Graphene-MCT Schottky diode detector

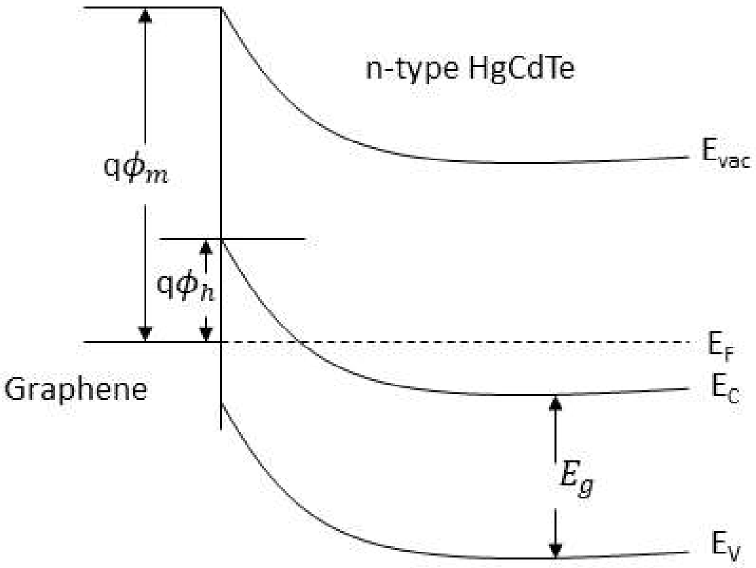

Fig.5.2 Energy band diagram of the proposed Schottky diode under equilibrium

Fig.5.2 shows the energy band diagram of the proposed device under equilibrium conditions. Under reverse bias conditions, the width of the depletion region increases, and the contact potential is increased by a factor of the applied reverse bias. As it is a majority carrier device, very less leakage current in the device is observed.

5.3 Numerical Simulation

The simulation of the Schottky diode detector is carried out using a two-dimensional numerical simulator, the Silvaco ATLAS TCAD tool. TCAD is useful to design, test, and optimize the Schottky diode detector ideas before actual device fabrication. It is a semiconductor simulator that has been used by industry and universities over the past few decades. It has a built-in database for common semiconductor material properties. The characteristics of exotic materials that are commonly used in advanced semiconductors can be manually inputted. When designing a Schottky diode detector, Silvaco ATLAS allows for easily modifiable dimensions and doping concentrations of each region. Underlying each region, the user defines a grid-based mesh. The mesh must be dense in the regions with rapidly varying carrier energy such as the depletion region, heterojunctions, electrodes, interfaces between different doping concentrations, and regions with differing refractive indices. For the current-voltage characteristics, the electrostatic Poisson’s equation together with continuity equations for electrons and holes have been solved. Thermionic emission theory has been considered for the electron-phonon interaction and the reduction of barrier height for the calculation of current-voltage characteristics. SILVACO Atlas uses Luminous to model light propagation and absorption within a device. One available Luminous physical model is Ray Tracing (RT) where light is treated as a point particle. RT is useful as it is not computationally expensive and hundreds of simulations can be done relatively quickly. The Luminous RT model uses an incident beam that is split into a series of rays that sum to cover the width of the simulated device. Based on the illumination profile, the simulator uses Newton's method to iteratively solve for the roots of the governing semiconductor non-linear differential equations at each grid point. It also solves for several other parameters, namely SRH recombination rate, auger recombination rate, radiative recombination rate, Fermi-Dirac statistic, electron and hole mobility based on doping concentration, and ohmic and Schottky contact interactions. We have employed the mechanism followed in the previous chapters for the simulation studies of the proposed device. The flow chart for the procedure of simulation has been presented in Fig.5.3.

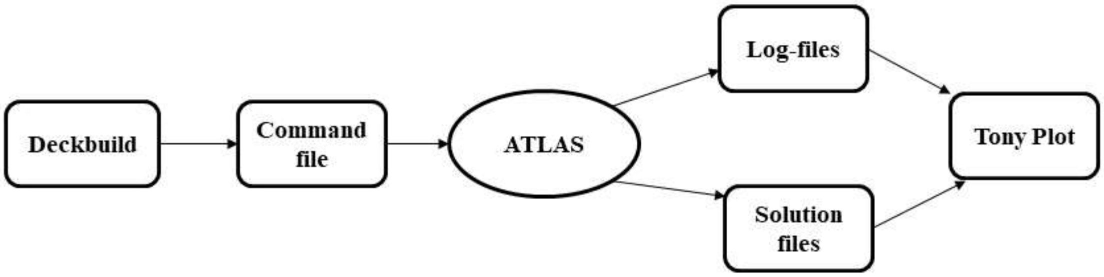

Fig.5.3 Flow chart for the simulation in ATLAS

5.4 Results and Discussion

The Schottky diode detector is designed and simulated in the commercially available TCAD tool ATLAS, Silvaco. The proposed device is characterized by electrical and optical characteristics. The thickness of the HgCdTe is taken of the order of 10 μm. The doping of the semiconductor is n-type of the order of $10^{22}\ /m^3$. The material parameters used have been discussed in the previous chapters. A THz radiation of optical power density of 10^4 W/m^2 is incident on the metal (graphene) contact. As the graphene layer is thin, there is a chance for less surface recombination taking place at the graphene surface and most of the radiation reaches the n-HgCdTe. Therefore, it is possible to generate a greater number of electron-hole pairs in the active region. Thus, it is possible to obtain enhanced optical characteristics in the proposed device in comparison to the conventional p-n diodes and p-i-n diodes. The following device physics has been employed in the numerical simulator for the device.

The work function of the MCT is calculated from the following expression

$$\phi_{HgCdTe}(eV) = \chi_{HgCdTe} + \frac{kT}{q}\ln\left(\frac{N_C}{N_D}\right) \tag{5.1}$$

where ϕ_{HgCdTe} is the work function of MCT, χ_{HgCdTe} is the electron affinity of MCT, k is the Boltzmann's constant, q is the electron charge, N_C is the effective density of electrons in the conduction band, and N_D is the donor concentration.

As graphene and MCT form a Schottky contact, a barrier would be developed at the point of contact. This barrier will prevent the diffusion of carriers (electrons) from the semiconductor to the metal. The height of the Schottky barrier is given by

$$\phi_h(eV) = \phi_{Gr} - \chi_{HgCdTe} \tag{5.2}$$

where ϕ_h is the height of the Schottky barrier, ϕ_{Gr} is the work function of graphene.

The built-in potential (V_{bi}) of the Schottky diode is given by

$$V_{bi} = \frac{\phi_{Gr} - \phi_{HgCdTe}}{q} \tag{5.3}$$

Since the graphene is extremely thin in the Schottky diode considered, the depletion region on the graphene is neglected. The depletion on the n-MCT is thick and is considered to be the depletion region of the Schottky diode. The expression for the width of the depletion region is given as

$$W = \left[\frac{2\epsilon(V_{bi} - V)}{qN_D}\right]^{\frac{1}{2}} \tag{5.4}$$

where W is the width of the depletion region, V is the applied bias voltage.

The current-voltage relationship in the Schottky diode is given by the thermionic emission theory.

$$I = I_o \exp\left(\frac{qV}{n_{idl}kT} - 1\right) \tag{5.5}$$

where n_{idl} (=2) is the ideality factor.

The reverse saturation current (I_o) is given by

$$I_o = AA^{**}\, T^2\, exp\left(-\frac{q\phi_h}{kT}\right) \tag{5.6}$$

Richardson's constant (A^{**}) is given by

$$A^{**} = \frac{4\pi q m^* k^2}{h^3} \tag{5.7}$$

By using the physics discussed in this section, numerical simulations have been performed and the following results are obtained.

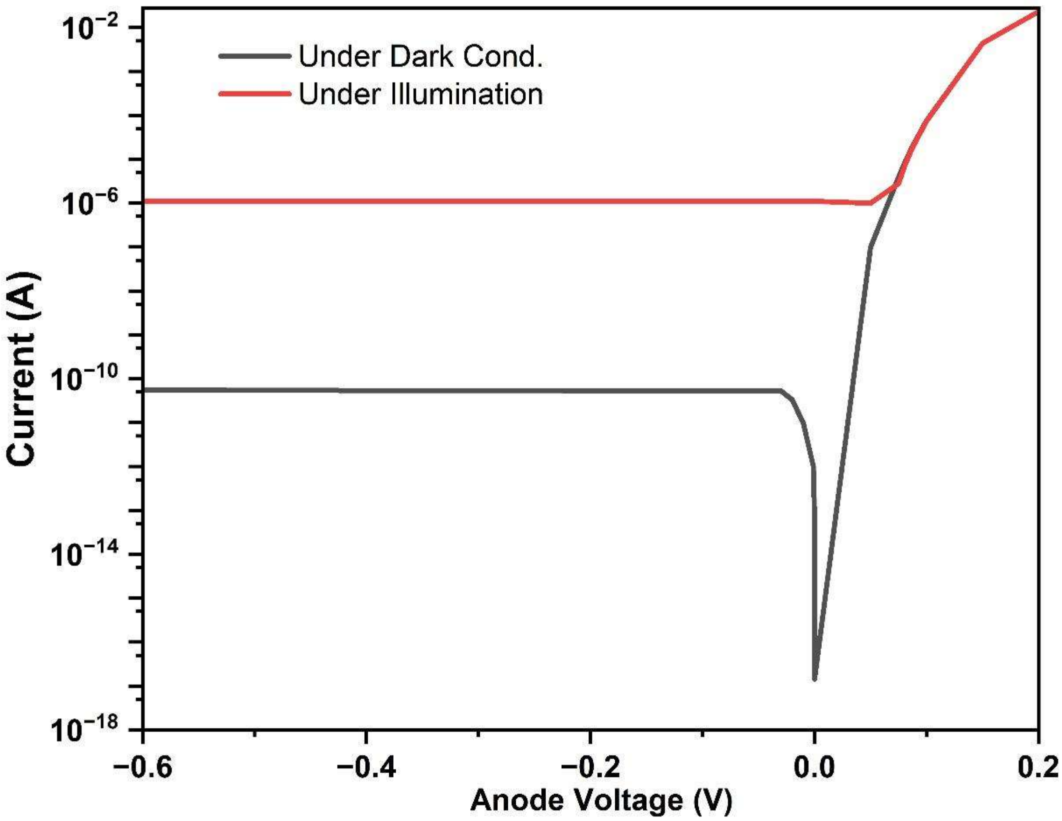

Fig.5.4 Variation of current under dark and illumination conditions for the applied voltage bias

The formation of Schottky between the metal contact (graphene) and HgCdTe results in a low dark current as it is a majority carrier device. From Fig.5.4, it can be concluded that under the illumination condition ($P_{opt}=10^4$ W/m^2), the current flowing in the device is more than the current under dark conditions.

The important figures of merit of a photodetector are quantum efficiency, responsivity, and specific detectivity. These have been discussed in the previous chapters. Here, only the variation of these parameters with the applied reverse bias of 0.5 V over a wavelength range has been shown. The analysis has been carried out with an incident optical power density of $P_{opt}=10^4$ W/m^2 on the device.

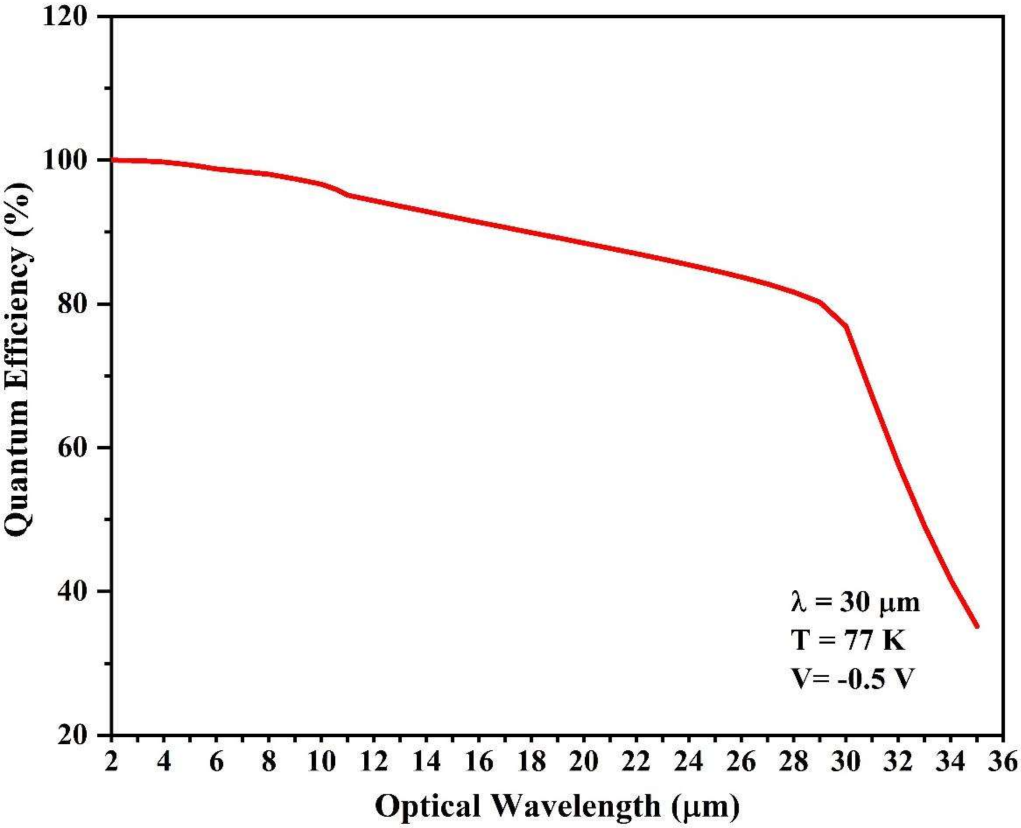

Fig.5.5 Variation of quantum efficiency with the wavelength at a reverse bias of 0.5 V

It is observed from Fig.5.5 that the Schottky diode detector exhibited a quantum efficiency of 77.87 %. The reason is that the thickness of the graphene is less, allowing more incident radiation to reach the depletion region. Thus, resulting in creating a greater number of electron-holes pairs (to be collected) than the n-i-p photodetectors proposed in the previous chapters. Therefore, resulting in better efficiency.

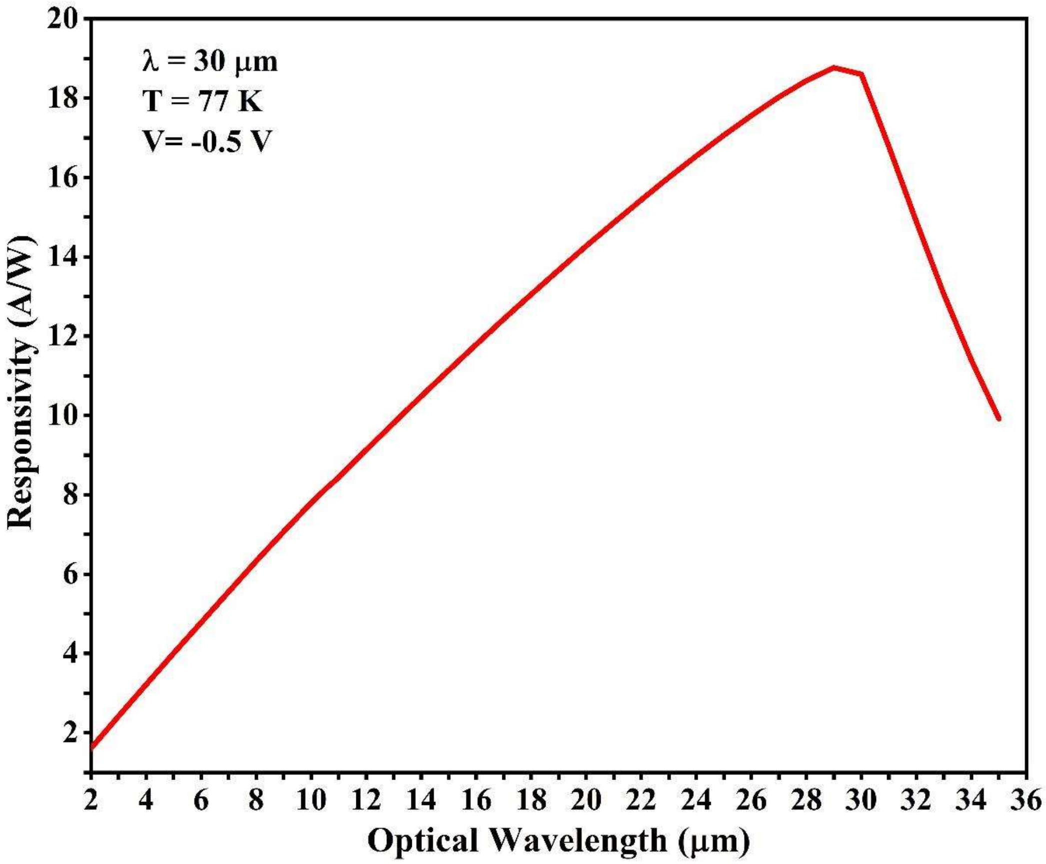

Fig.5.6 Variation of responsivity with the wavelength at a reverse bias of 0.5 V

It can be seen from Fig.5.6 that the Schottky diode detector exhibited a responsivity of 18.6 A/W. The responsivity of the proposed device is more than the values reported in chapter 3 and chapter 4.

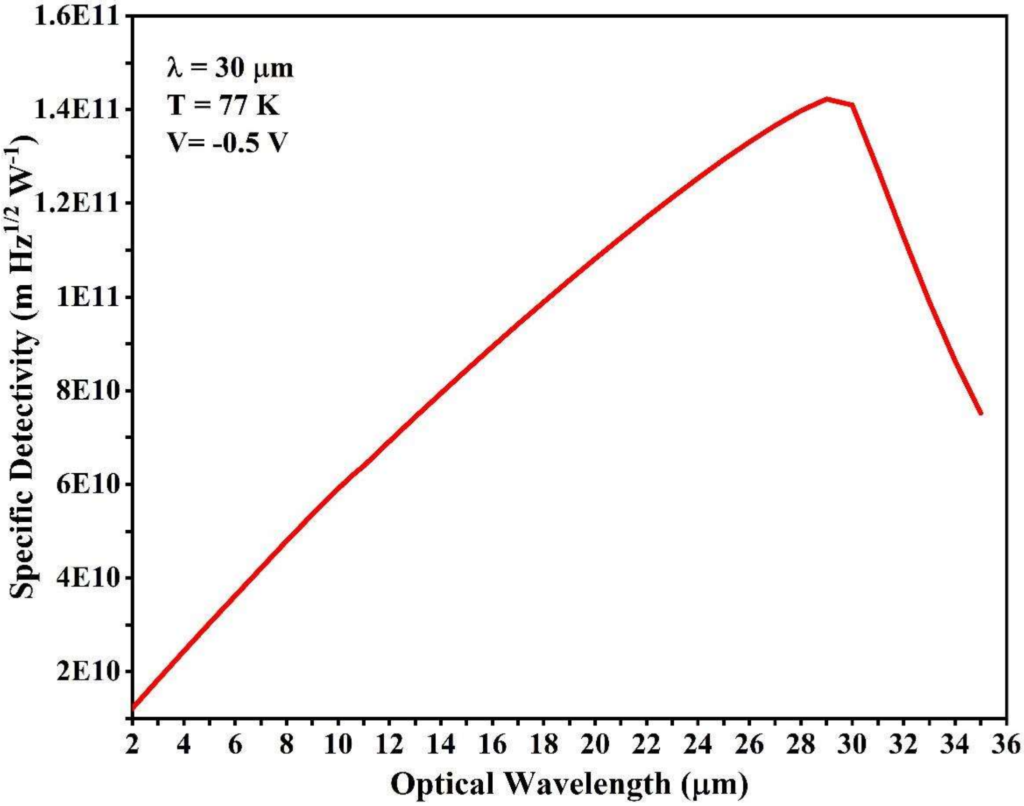

Fig.5.7 Variation of specific detectivity with the wavelength at a reverse bias of 0.5 V

It is observed from Fig.5.7 that the Schottky diode detector exhibited a specific detectivity of $1.40 \times 10^{11}\ mHz^{1/2}W^{-1}$. The specific detectivity depends on the dark current. The dark current is less in the case of the Schottky diode detector due to its structural advantage. Thus, we can observe that the specific detectivity is more than the values reported by single heterojunctions and double heterojunctions reported in chapter 3 and chapter 4 respectively.

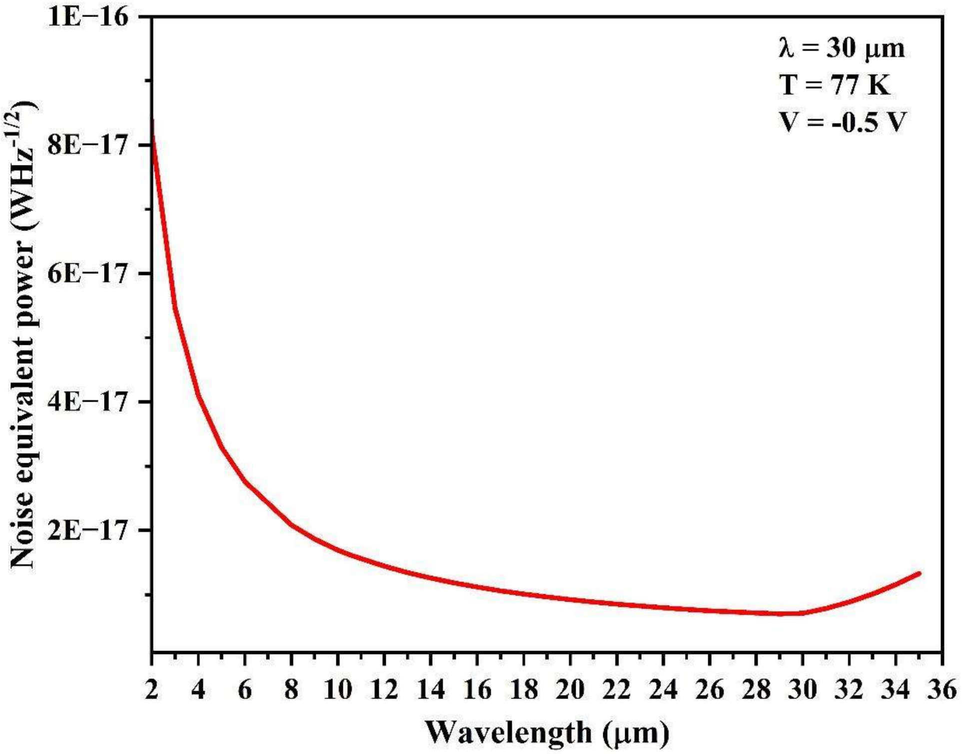

Fig.5.8 Variation of NEP with the wavelength at a reverse bias of 0.5 V

It is observed from Fig.5.8 that the Schottky diode detector exhibited a NEP of $0.71 \text{ x } 10^{-17}\ WHz^{-1/2}$. The NEP of the proposed device is less than the reported values of n-i-p photodetectors in the previous chapters. Hence, it can be concluded that the Schottky diode detector designed performs better than the n-i-p photodetectors.

Table 5.1 compares the responsivities of various graphene-based photodetectors reported in the literature. It is found that the proposed device exhibits an improved value of responsivity in comparison to the other graphene-based photodetectors.

Table 5.1 Performance of the graphene-based photodetectors

Device	Responsivity (A/W)	Reference
Graphene/Si	0.73	[167]
Graphene/Si	0.73	[168]
Graphene/Si	0.23	[169]
Graphene/Si	0.435	[170]
Graphene/Si	0.140	[171]
Graphene/Si	0.214	[172]
Graphene/Si	0.152	[173]
Graphene/Si	0.142	[174]
Graphene/Si	0.24	[175]
Gr/Si-tips junction	2.5	[176]
Graphene/metal	0.225	[177]
Graphene/Ge	0.0518	[178]
Graphene/HgCdTe	18.6	This work

Table 5.2 shows the comparison of the detector’s performance of the devices reported in this thesis. It can be concluded that the proposed detectors outperform the n-i-p photodetectors reported in the previous chapters.

Table 5.2 Comparison of the detectors

Parameter	Single Heterojunction [134]	Dual Heterojunction [179]	Schottky Barrier Detector (Proposed)
Current under Dark Condition (A)	$4.6 \text{ x } 10^{-9}$	$2.6 \text{ x } 10^{-10}$	$5.4 \text{ x } 10^{-11}$
Quantum Efficiency (%)	73.93	75.35	77.88
Responsivity (A/W)	17.9	18.21	18.6
Specific Detectivity (mHz$^{1/2}$W^{-1})	$1.44 \text{ x } 10^{9}$	$1.99 \text{ x } 10^{9}$	$1.41 \text{ x } 10^{11}$
Noise Equivalent Power (WHz$^{-1/2}$)	$0.3 \text{ x } 10^{-16}$	$0.21 \text{ x } 10^{-16}$	$0.71 \text{ x } 10^{-17}$

5.5 Conclusion

This chapter studies the performance of a Schottky diode detector for the absorption wavelength of 30 μm through simulation in the ATLAS Silvaco TCAD tool. The proposed device utilizes the high transmittance property of graphene which aids in incident THz radiation reaching the semiconductor region with very less absorption in graphene. The optical characteristics obtained are encouraging and the device delivered a low dark current. Overall, the Schottky diode detector proposed exhibited enhanced optoelectronic characteristics compared to the photodetectors reported in the previous chapters.