

# Self consistent carrier transport in band engineered HgCdTe nBn detector

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**Abstract**—In this paper we study the influence of carrier transport under non-equilibrium condition in HgCdTe superlattice barrier detector employing self-consistent NEGF-Poisson solver. We use single-band effective mass approximation extracted from  $k,p$  envelope function to calculate dark current in the presence of applied bias. We expect the properties of superlattice barrier (doping, layer width, etc.) modify the band alignment between barrier layer and absorber layer, and consequently the dark current of band engineered HgCdTe detector will vary.

**Keywords**—HgCdTe nBn detector; superlattice barrier; band engineering; styling; NEGF; carrier transport.

## I. INTRODUCTION

In recent years the concept of HgCdTe nBn infrared detector has gained huge attention as an alternative to the traditional photovoltaic detector design. However, such a detector design requires a large reverse bias in order to operate properly due to existence of the valence band discontinuity ( $\Delta E_v$ ) and, therefore, severe degradation in the performance of the detector will be observed [1,2]. Different approaches have been recently proposed by ND Akhavan *et. al.* to eliminate the valence band discontinuity in HgCdTe nBn detectors. These methods are based on engineering the barrier layer of the HgCdTe nBn detector in order to align the position of valence band between barrier layer and absorber layer of the detector and are referred to as “band engineering” technique in general [3,4]. Figure 1a shows the conventional HgCdTe nBn detector where the valence band offset impedes the flow of carrier from absorber towards contact layer. Figure 1b shows the band engineered HgCdTe where the valence band discontinuity has been removed using one of the available methods. Among

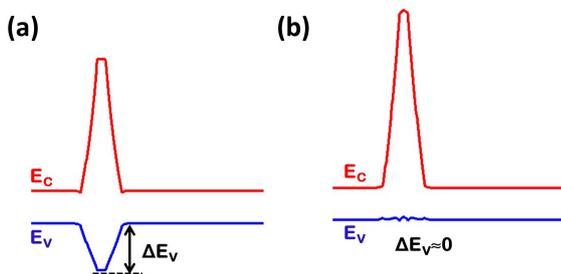


Fig. 1. (a) Conventional nBn detector and, (b) band engineered nBn detector where valence band discontinuity has been removed.

different band engineering methods, superlattice barrier technique is superior to the other methods since it does not involve p-type doping of the barrier layer. The schematical representation of the superlattice barrier is shown in Figure 2 where the barrier layer of this detector design is composed of periodic replication of CdTe-HgTe-CdTe quantum well. Such a barrier design results in discrete energy levels in conduction band and valence band of the barrier region. The ultimate goal of superlattice barrier is to design the superlattice in order to achieve maximum difference between absorber/superlattice conduction band, and minimum difference between absorber/superlattice valence band.

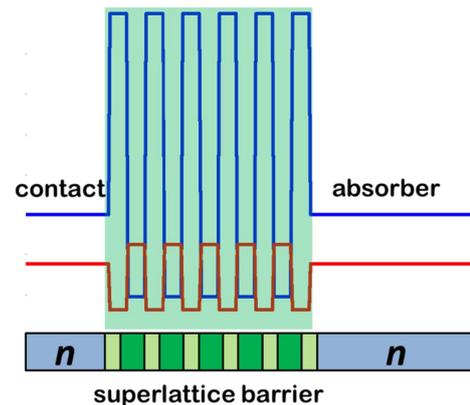


Fig. 2. HgCdTe nBn detector with superlattice barrier design.

## II. MODELLING APPROACH

In order to calculate the band structure and carrier transport in HgCdTe nBn detector with superlattice barrier, we employ the non-equilibrium Green’s function (NEGF) formalism, solved self-consistently with Poisson equation. This approach is the most valid theoretical method which has been successfully used to study the carrier transport in different low-dimensional structures such as nanowire FETs, III-V materials and p-n photodiode [5, 6]. Figure 3 shows the flowchart of NEGF-Poisson solver which is used in this study. The main equations for NEGF formalism are as follows:

$$G = (EI - H - \Sigma_R - \Sigma_L) \quad (1)$$

$$G^< = G \Sigma^< G^+ \quad (2)$$

$$T = \text{trace}(G\Gamma_L G^+\Gamma_R) \quad (3)$$

where  $G$  and  $G^<$  are the retarded and lesser Green's functions, respectively.  $T$  is the transmission probability of carriers from left side of detector to the right side of the detector. The definition of these elements can be found in literatures [5]. The electronic structure HgCdTe is calculated using the one-band effective mass approximation where the electron-hole effective masses are extracted from the  $8 \times 8$  k.p envelope function around the  $\Gamma$  point of the band structure. Figure 4 shows the effective masses of electrons and heavy holes for HgTe and CdTe. The effective mass of HgCdTe is calculated by linear interpolation of parameters between HgTe and CdTe. Figure 5 shows the transmission probability versus energy which is an indication of band alignment in HgCdTe nBn detector. The coupling between NEGF-Poisson which takes into account the doping density of each layer is not considered here and will be shown in the future.

Acknowledgments

This work is funded by the Australian Research Council under, the Discovery Project program (DP120104835) and Australian National Fabrication Facility (ANFF).

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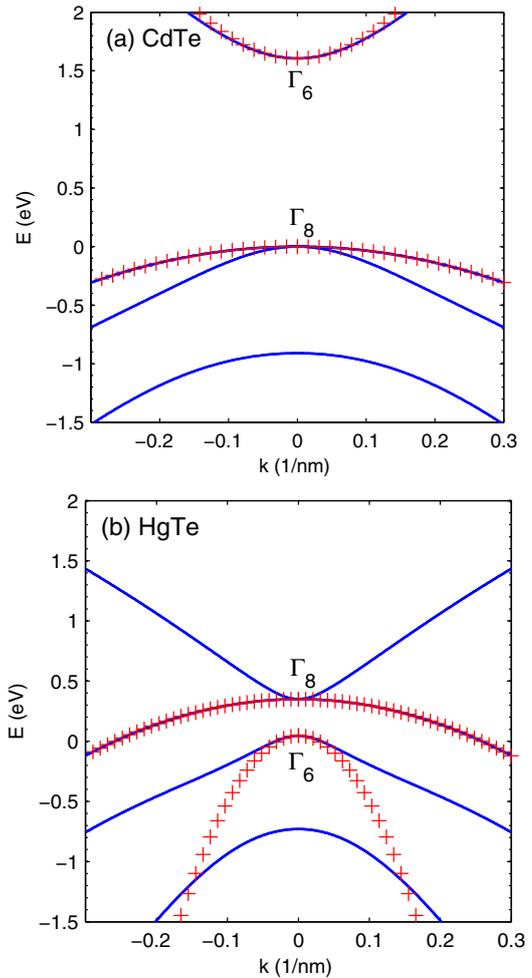


Fig. 4. Extraction of effective mass from  $8 \times 8$  k.p envelope function. (a) for CdTe with normal band structure, and (b) HgTe with inverted band structure.

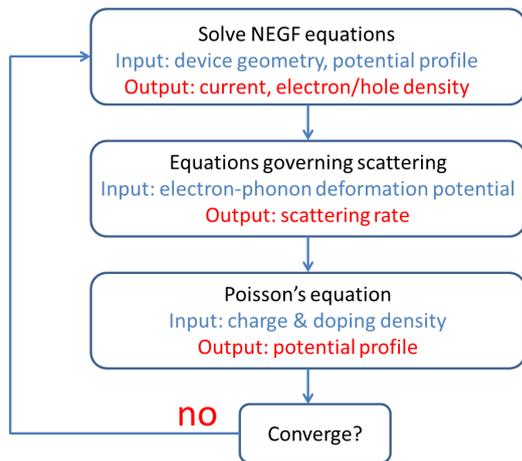


Fig. 3. Flowchart of NEGF-Poisson solver algorithm. After convergence, charge distribution, potential profile and current density are obtained.

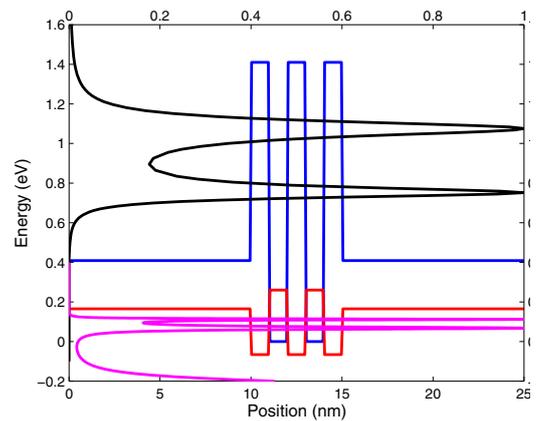


Fig. 5. Transmission probability at different energy levels for superlattice barrier HgCdTe nBn detector. The superlattice is undoped with CdTe layer width of 1nm and HgTe layer width of 1nm. For this particular arrangement, the electrons can easily tunnel from left side of detector to the right side of detector which results in high dark current density.