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Insights on energy selective contacts for thermal energy harvesting using double resonant tunneling contacts and numerical modeling

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ABSTRACT

Energy selective electrical contacts have been proposed as a way to approach ultimate efficiencies both for thermoelectric and photovoltaic devices as they allow a reduction of the entropy production during the energy conversion process. A self-consistent numerical model based on the transfer matrix approach in the effective mass and envelope function approximation has been developed to calculate the electronic properties of double resonant tunneling barriers used as energy selective contacts in hot carrier solar cells. It is found that the application of an external electric bias significantly degrades the electronic transmission of the structure, and thus the tunneling current in the current-voltage characteristic. This is due to a symmetry breaking which can be offset using finely tuned asymmetric double resonant tunneling barriers, leading to a full recovery of the tunneling current in our model. Moreover, we model the heterostructure using electrons temperature in the emitter higher than that of the lattice, providing insights on the interpretation of experimental devices functioning in hot carrier conditions, especially regarding the previously reported shift of the resonance peak (negative differential resistance), which we interpret as related to a shift in the hot electron distribution while the maximum remains at the conduction band edge of the emitter. Finally, experimental results are presented using asymmetric structure showing significantly improved resonant properties at room temperature with very sharp negative differential resistance.

1. Introduction

As energy conversion occurs, a sizeable fraction gets converted to incoherent, thermal, energy, following the second principle of thermodynamics. This is why thermal energy is widely available, but unfortunately its efficient conversion to electricity has been elusive. With the advent of nanostructured materials, new efficient pathways have emerged [1,2], that may prove useful both for pure thermoelectric conversion as well as for mixed thermal/photovoltaic conversion [3] as in hot carrier solar cells.

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The concept of hot carrier solar cells (HCSC) has been introduced since the early 1980's by Ross and Nozik [3], however a fully functioning proof-of-concept device is yet to be realized as major technological locks still exist. A HCSC combines a slow carrier cooling absorber limiting the interaction between phonons and photocarriers, and energy selective contacts (ESC) extracting the photocarriers at a specific energy higher than the band edge; as researches concerning the absorber part have steadily progressed bringing interesting new results at a steady pace in the past decades [4–8], the work on ESC remains quite limited both on the theoretical and experimental aspects [9–12]. Among the different concepts that have been proposed to achieve energy selectivity, the use of double resonant tunneling barriers (DRTB) [13] is a very promising design as such heterostructures are now well controlled experimentally, while already well known from their applications in resonant tunneling diodes [13–15], and different groups working on HCSC have performed experiments using DRTB to demonstrate their potential application as ESC [16–19]. Takeda's group recently investigated on the conductivity of a DRTB-type ESC and showed that such heterostructure are potentially suitable to be used in a realistic device; however, as HCSC are supposed to work under electric bias, the symmetry breaking of the electrostatic potential resulting from the application of the polarization could lead to a strong degradation of the transmission of the DRTB, hindering the collection of generated hot carriers. As a result, the correct interpretation of the J-V curve for a proof of concept ESC might become somewhat problematic and modeling such a structure functioning with hot carriers provides us with insights on the correct interpretation of experimental data. Specifically, ESC can be seen as thermoelectric machines for which it is possible to calculate a Seebeck coefficient from the electronic transmission of the contact [2,20], and in that context, an understanding at the fundamental level of the DRTB transport properties is extremely valuable.

In this work, we first address the issue of maintaining a maximum transmission for a DRTB acting as an ESC under electric bias using computer simulation. Our model is based on the transfer matrix method [21] in the approximation of the effective mass and the envelope function. Our approach was to offset the symmetry breaking from the electric bias by using asymmetric barriers which restores a maximum transmission for electron resonant tunneling. The concept of “effective-barrier symmetry” has been introduced by Mendez [22] and discussed for DRTB by Allen [23]. Very recently, asymmetric structures using a GaN substrate have been modeled using an InGaN well on the collector side [24], though only theoretical results have been presented. While our work has the same basis, we focus here on the application of such heterostructure to HCSC by introducing an electron temperature and self-consistency in the model to evaluate the space charge effects on the electronic transport, resulting in a qualitative description closer to the experimental characterization of such a device functioning with an actual hot carrier extraction.

A brief introduction to the model, its possibilities and its limitations will be given, then we will model the electronic transport in a DRTB and study the influence of the electric bias while a barrier asymmetry will be shown to fully recover the maximum electronic transmission of the DRTB. The J-V characteristic of the device will be modeled and its important features described focusing on the importance of using a self-consistent model to accurately describe a realistic DRTB. By introducing an electrons temperature on the emitter side of the heterostructure, we will discuss on the evolution of the J-V characteristic and the implication for the experimental detection of hot carriers passing through the resonant state of the DRTB. Finally, experimental characterization of symmetric and asymmetric DRTB will be presented supporting the conclusions from the model.

2. Model description, limitations

2.1. Description

The goal of this model is to calculated the electronic transmission of a DRTB under electric bias, and the J-V characteristic of such heterostructure by using material parameters and a user-defined carrier density/temperature quasi-fermi level as in input in the emitter and collector. The model is coded using Python, and is based on a transfer matrix approach [21,23], in the effective mass and envelope function approximations, where the time independent Schrodinger's equation is solved through the DRTB using boundary conditions at each interface. Our model focuses on GaAs/AlGaAs heterostructures as their nearly identical lattice parameter makes this system an interesting candidate for experimental realization of DRTBs, but the method could easily be transferred to other systems as the three main bulk parameters taken as input are the band offset, the effective mass and the dielectric constant. The propagation of an incident electron in the z-direction (1D confinement) is obtained by solving the time independent Schrodinger's equation using the BenDaniel-Duke boundary conditions [25,26], which state the continuity of $\psi(z)$ and $\frac{1}{m^*}\frac{\partial\psi(z)}{\partial z}$ where m^* is the effective mass of the electron and $\psi(z)$ the z-component of the wave function. Using these boundary conditions in an arbitrary heterostructure such as on Fig. 1 a, 4 transfer matrices are obtained, and considering that no electron is coming from the collector side, it is possible to obtain the transmission T and reflection R probabilities of the DRTB:

$$R = \left|\frac{(M_t)_{2,1}}{(M_t)_{2,2}}\right|^2 \text{ and } T = \frac{k_5}{k_1}\frac{m_1^*}{m_5^*}\left|(M_t)_{1,1} - \frac{(M_t)_{2,1}(M_t)_{1,2}}{(M_t)_{2,2}}\right|^2 \quad (1)$$

where $M_t = M_{4\rightarrow5}\cdot M_{3\rightarrow4}\cdot M_{2\rightarrow3}\cdot M_{1\rightarrow2}$ are the transfer matrixes at each interface and $k_j = \frac{\sqrt{2m_j^*(E_Z - V_j)}}{\hbar}$.