Monte Carlo simulation of solid-state thermionic energy conversion devices based on non-planar heterostructure interfaces

Z. Bian, A. Shakouri

Electrical Engineering Department, University of California Santa Cruz,
Santa Cruz, CA 95064

Summary. In this paper, electron emission from non-planar potential barrier structures is analyzed using a Monte Carlo electron transport model. Compared to the planar structures, about twice bigger emission current can be achieved for the non-planar tall barriers. The thermionic emission enhancement is attributed to combined effects of increased effective interface area and reduced probability of total internal reflection at the heterostructure interface.

1 Introduction

Heterostructure integrated thermionic devices are expected to offer larger thermoelectric power factor by selective emission of hot electrons while keeping similar electrical conductivity as the highly degenerate emitter material.[1, 2] However, it has been shown that the improvement in efficiency due to enhanced electronic transport properties is limited.[3] The main shortcoming of planar barriers is that they only transmit “hot” electrons whose kinetic energy in the direction perpendicular to the barrier is large enough. In this paper, we show that it is possible to increase the number of electrons contributing to the electrical conductivity by using non-planar potential barriers. A schematic of a heterostructure thermionic device with zigzagged interface is shown in Fig. 1. Electrons in a larger volume of the momentum space can be emitted due to multiple tilted directions of the barrier. In the real space, the effective interface area is increased for zigzagged structures. However, an electron that crosses the interface may reenter the emitter region in a rough heterostructure even without any scattering. On the other hand, an electron that is reflected from the barrier by total internal reflection may hit the next barrier surface with smaller angle with respect to normal. As it can be seen in Fig. 2, more electrons have a chance to pass over the barrier in a triangle region.

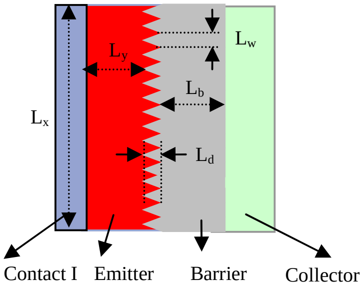

Fig. 1. A solid-state thermionic device with non-planar potential barrier.

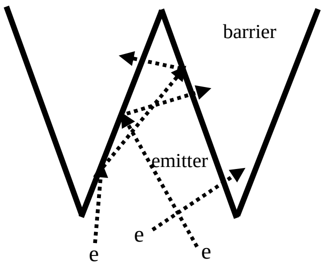

Fig. 2. Illustration of electron trajectories.

2 Monte Carlo Algorithms

We used a simplified ensemble Monte Carlo model to simulate the transport of a two-dimensional electron gas across a two-dimensional non-planar potential barrier. We included the random inelastic scattering in the Monte Carlo method which reassigns a random momentum to the scattered particle according to Fermi-Dirac statistics. In this way, the electron temperature was kept the same as the lattice temperature at the operation condition. The electron scattering was modeled with a constant relaxation time 88.5 fs for InGaAs material and the estimated electron mean-free-path was 0.188 µm for Fermi energy 526 meV. Since the mean-free-path is small at high doping densities and the electron wave generally loses coherence in the barrier, quantum mechanical interference and transmission are neglected. The simulation focuses on the effects of non-planar barrier; thus, a uniform barrier height of 500 meV was used, rather than a self-consistent band bending calculation. This will not change the results significantly because the emitter is much bigger than the interface region and energy distribution of electrons are mostly determined by the bulk emitter. A constant time step of 2 fs was used, which is much less than the scattering relaxation time. The carrier distribution at the quasi-equilibrium state is shown in Fig. 3. The zigzag interface can be clearly seen. Fig. 4 shows the energy distribution of the electrons along the structure. The hot electron filtering of the barrier structure can be clearly seen.

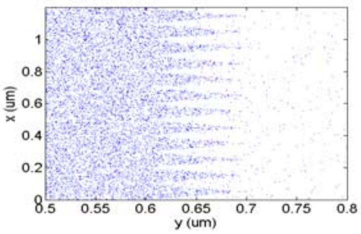

Fig. 3. Electron distribution in real space.

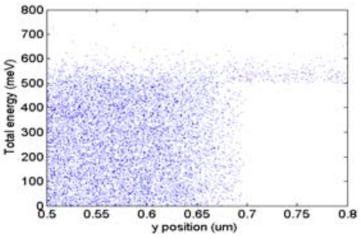

Fig. 4. Electron energy distribution along y direction

3 Simulation Results

Regardless of energy, the total current improvement for the zigzag non-planar barrier compared to that of the planar barrier (with width L_b+L_d/2) is shown in Fig. 5. It can be seen that the emitted current increases with the increase of depth L_d or the decrease of the period L_w. The dependence on period is easily understood since a larger period is related to a smaller effective interface area and the two regions in the momentum space have larger overlap. These two regions represent emitted electrons with enough kinetic energy perpendicular to each section of the barrier. An increase of the zigzag depth makes the affective interface area larger. However, when period L_w is small, emitted electrons have more chance to go back to the emitter region for a large zigzag depth. Thus, the improvement converges to an enhancement factor of 1.73 at small periods and large depths.

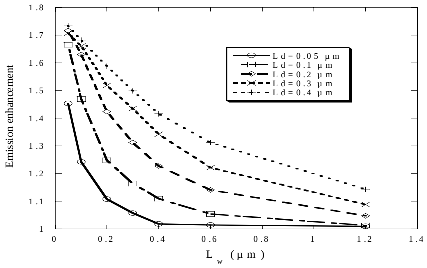

Fig. 5. The current enhancement as a function of zigzag dimensions.

The chance to have a larger total back-scattering and smaller transmission from a non-planar interface is small. One expects more current emission enhancement from more complex interface geometries. Fig. 6 shows a zigzag interface with four tilted directions. The zigzag period L_w is divided evenly into four sections; and the zigzag depth is divided to two sections with the ratio of 1:2. The Monte Carlo simulation results of geometry dependence are shown in Fig. 7. Similar dependences on the zigzag period and depth as for the two-direction zigzag case can be seen. A factor of 2 maximum improvement compared to planar barriers has been achieved for small periods and large depths. One should note that at very small zigzag periods, when the feature size is smaller than the electron de Broglie wavelength (~8 nm), electrons will see an “effective” barrier profile. In this case a more accurate analysis should use 2D Schrodinger equation and calculate the quantum mechanical transmission coefficient. The overall improvement in the number of emitted electrons will persist as long as a larger volume of electrons in the momentum space can participate in the thermionic emission. [4]

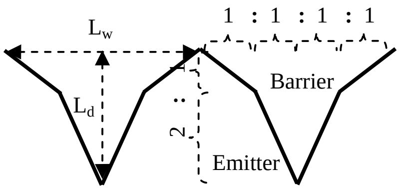

Fig. 6. Illustration of the 4-direction zigzagged interface

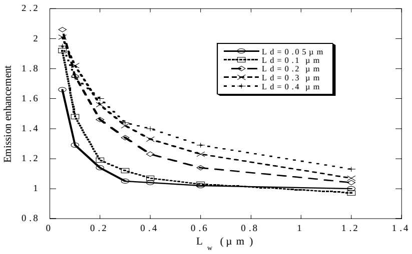

Fig. 7. The current enhancement of the 4-direction zigzag.

4 Conclusions

Non-planar heterostructure potential barriers can increase the number of electrons thermally emitted above the barrier. A factor of 2 of emission enhancement can be achieved with a 4-direction zigzagged barrier.

5 Acknowledgements

The authors thank Professor U. Ravaioli at UIUC for valuable suggestions.

References

1. A. Shakouri and J. Bowers, Appl. Phys. Lett. **71**, 1234 (1997).
2. G. D. Mahan and L. M. Woods, Phys. Rev. Lett. **80**, 4016 (1998).
3. M. D. Ulrich, P. A. Barnes, and C. B. Vining, J. Appl. Phys. **90**, 1625 (2001).
4. D. Vashaee and A. Shakouri, Phys. Rev. Lett. **92**, 106106 (2004).