Enhanced solid-state thermionic emission in nonplanar heterostructures

Zhixi Bian and Ali Shakouri[a)]
Baskin School of Engineering, University of California, Santa Cruz, California 95064

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Conservation of transverse momentum during thermionic emission from planar structures is a key factor limiting the number of hot electrons emitted and the efficiency of solid-state thermionic energy conversion devices. In this letter, electron emission from nonplanar potential barrier structures is analyzed using a Monte Carlo transport model. Compared to the planar structures, nonplanar tall barriers can achieve much larger emission currents. Although the average energy of the transmitted electrons drops a little, the thermoelectric figure of merit can be increased with a nonplanar barrier structure. The improvement of the thermoelectric properties is attributed to the combined effects of increased effective interface area and reduced probability of total internal reflection at heterostructure interfaces. © *2006 American Institute of Physics*.
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The performance of a thermoelectric device is mostly determined by the dimensionless figure of merit ZT. ZT is defined as $ZT=(S^2\sigma/k)T$, where T is the absolute temperature, S is the Seebeck coefficient, and σ and k are the electrical and thermal conductivities, respectively.[1] Heterostructure devices based on thermionic emission are expected to offer a larger thermoelectric power factor ($S^2\sigma$) than bulk materials due to the increase in the Seebeck coefficient by selective emission of hot electrons while maintaining a similar electrical conductivity as highly degenerate materials.[2,3] However, it has been shown that such an enhancing technique can only improve the thermoelectric properties slightly.[4] Instead, the advantage of conventional planar superlattices or multilayers is in the reduction of phonon transport and the parasitic heat loss.[5,6] The main shortcoming of planar barriers is that they only transmit electrons whose kinetic energy in the direction perpendicular to the barrier is large enough. Many other "hot" electrons with large in-plane momentum and large total kinetic energy are blocked by the potential barrier, resulting in a low electrical conductivity. To overcome this limitation, we proposed to use controlled roughness at the heterostructure interfaces to break the in-plane translational invariance and lateral momentum conservation. In this way, many more electrons with enough "total" kinetic energy are expected to contribute to the current transport.[7] The nonepitaxial interface scattering and lateral momentum nonconservation have been verified by ballistic electron emission microscopy for some metal/semiconductor interfaces.[8,9] However, the thermionic emission current enhancement needs to be further quantified for these experiments.

In this letter, we apply a nonplanar barrier to increase the probability of electron emission. A schematic of the heterostructure thermionic device with the zigzagged interface is shown in Fig. 1(a). Even though the lateral momentum in the plane of local interface is conserved, the wave vector space of useful electrons in the emitter becomes larger due to the multiple tilted directions of the barrier. In real space, the effective interface area is increased for zigzagged structures. The conductivity enhancement of the enlarged interface area of the rough barrier surface was addressed for metal-semiconductor contact in Ref. 10. However, the enhancement model was too simple and the enhancement factor was overestimated, because the length scale of the roughness relative to the electron mean-free-path was not considered. An electron that crosses the interface may re-enter 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 a smaller angle with respect to normal. As can be seen in Fig. 1(b), more electrons have a chance to pass over the barrier in a triangle region. One such nonplanar structure is the GaN pyramid array fabricated by selective growth.[11]

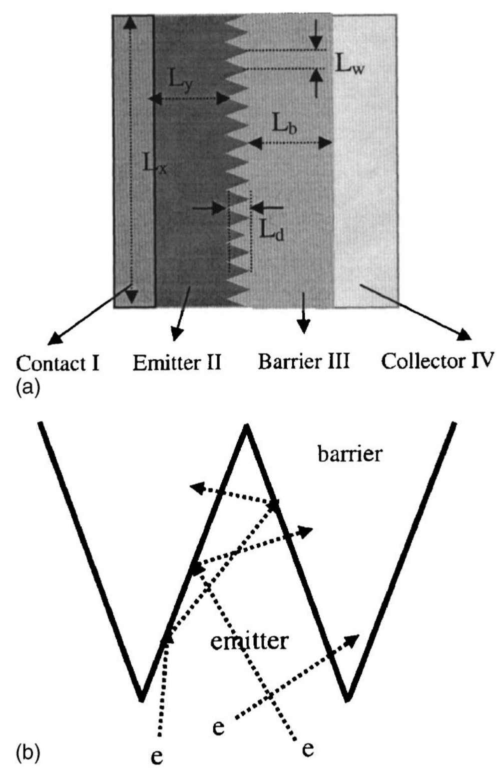

FIG. 1. (a) Schematic of a solid-state thermionic device with nonplanar potential barrier. (b) Illustration of electron trajectory in the interface region.

[a)]Author to whom correspondence should be addressed; electronic mail: ali@soe.ucsc.edu

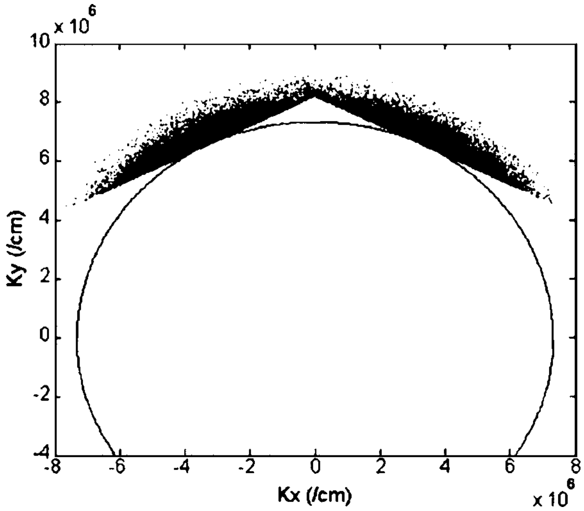

FIG. 2. Emitted electrons in the wave vector space for the two-direction zigzag with a period L_w of 0.4 μm and a depth L_d of 0.1 μm.

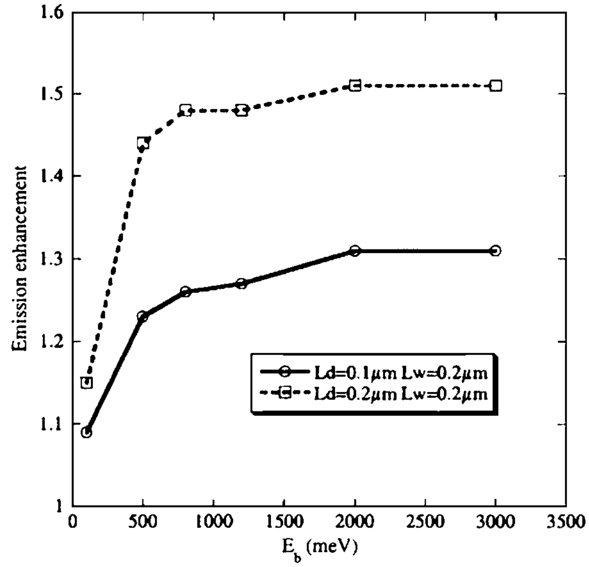

FIG. 4. The potential barrier height dependence of the current enhancement for nonplanar barriers.

We used a simplified ensemble Monte Carlo model to simulate the in-plane transport of a two-dimensional electron gas across a two-dimensional nonplanar potential barrier. A contact layer was introduced to supply electrons and keep a constant emission current. The material of the contact layer was the same as the emitter and the number of charge particles in the contact layer was kept constant. A total of 40 000 electron particles were assigned with random position and wave vector k_x and k_y according to Fermi–Dirac statistics. The collector worked as a perfect absorber, thus the unidirectional electron transport was investigated. When one electron was transported from the emitter to the barrier, it could have passed the interface only if its kinetic energy, in the direction of local normal, was larger than the barrier height. The enclosed surface of the whole structure was set as a total reflection mirror. We included the random inelastic scattering in the Monte Carlo method, which reassigned 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. 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. In the simulation domain, the emitter width L_x and length L_y were 1.2 μm and 1 μm, respectively. The barrier width excluding the zigzagged region was represented by L_b [see Fig. 1(a)] and was kept at 0.1 μm. A constant time step of 2 fs was used, which is much less than the scattering relaxation time. The particle number of unidirectional thermionic emission was counted for a period of 30 ps after the emission became stable.

Figure 2 shows an example of the emitted electrons in the wave vector space for a zigzag period L_w of 0.4 μm and a depth L_d of 0.1 μm. The circle with radius equal to wavevector length k_b corresponds to the barrier height E_b. For parabolic and sphere-symmetry band approximation, we have $E_b=\hbar^2k_b^2/2m^*$, where $\hbar$ and m^* are the reduced Planck constant and electron effective mass, respectively. It can be seen that electrons from two regions in the momentum space contribute to the current. These correspond to the two tilted directions of the barrier.

We changed the period L_w and depth L_d and the current improvement of the zigzag nonplanar barrier over the planar barrier (with width $L_b+L_d/2$) is shown in Fig. 3. It can be seen that the emitted current increases with the 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. An increase of the zigzag depth makes the effective interface area larger. However, when the period L_w is small, emitted electrons have a greater chance to

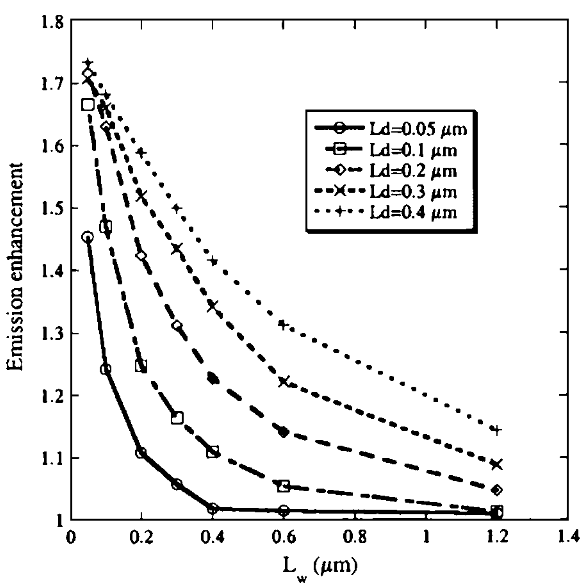

FIG. 3. The period and depth dependences of the current enhancement for the two-direction zigzag.

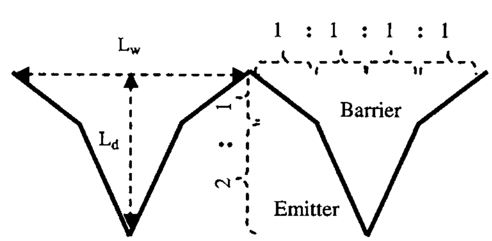

FIG. 5. Illustration of the four-direction zigzagged interface.

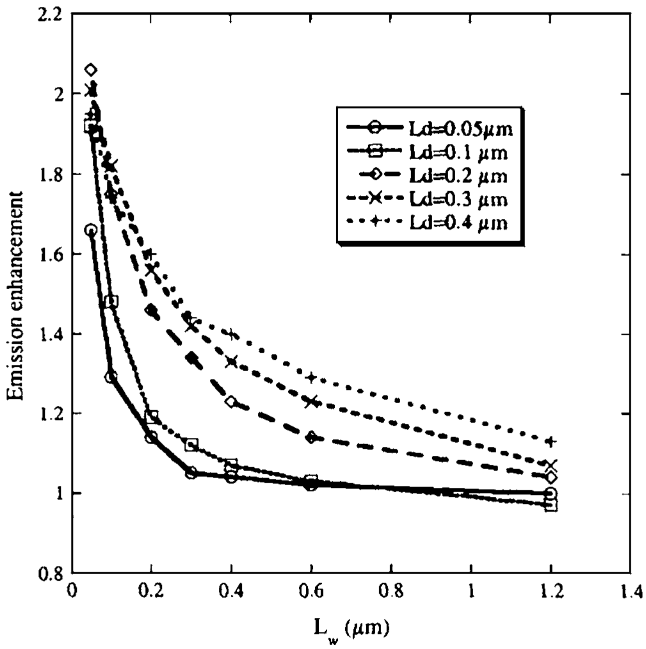

FIG. 6. The period and depth dependences of the current enhancement for the four-direction zigzag.

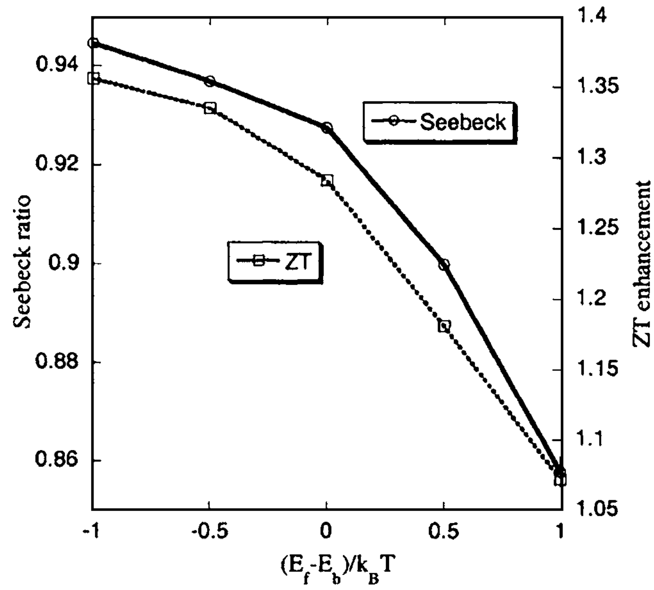

FIG. 7. The ratio of the Seebeck coefficients of the non-planar barrier and its planar counterpart and the *ZT* enhancement of the nonplanar barrier vs the reduced Fermi energy of the barrier.

go back to the emitter region for a larger zigzag depth. Thus, the improvement converges to an enhancement factor of 1.73 at small periods and large depths. It should be noted that the de Broglie wavelength of electrons at the Fermi level is about 8 nm and the decrease of the period is limited by the quantum mechanical wave nature of electrons. At very small feature sizes, electrons see only an effective planar interface. The increase of the zigzag depth is also restrained by the uniformity of local electrical field and temperature.

When regions of different directions in the momentum space can be used for electron emission, a taller barrier with the same reduced Fermi energy $(E_f - E_b)/k_B T$ is expected to give larger current because the overlap between different regions decreases. The barrier height dependence is shown in Fig. 4 for two different dimensions. It can be seen that there is a big increase in emission current when the barrier height changes from 100 meV to 500 meV, and the current improvement is saturated at high barrier heights.

One expects larger current emission enhancement from a zigzagged interface having more than two tilted directions. Figure 5 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 into two sections with the aspect ratio of 1:2. We varied the zigzag period and depth while keeping the aspect ratios the same in the tilted sections. A barrier height of 500 meV was used. Monte Carlo simulation results are shown in Fig. 6. Compared to planar barriers, an improvement in emission current by a factor of 2 can been achieved for small periods ($\sim$0.05 μm) and large depths ($\sim$0.3 μm).

The Seebeck coefficient of the thermionic heterostructure is proportional to the difference of the average energy of emitted electrons and the Fermi energy. The simulation showed that the Seebeck coefficient depends on the reduced Fermi energy of the barrier $(E_f - E_b)/k_B T$ very much. The simulation results are plotted in Fig. 7 for a four-direction zigzag with a period of 0.1 μm, a depth of 0.1 μm, and a barrier height of 500 meV. It can be seen that the ratio of the Seebeck coefficients of the nonplanar barrier and its planar counterpart decreases with the increase of the reduced Fermi energy. We assumed that the thermal conductivity was the same for planar and nonplanar barriers and the figure of merit *ZT* could be compared for the two cases according to the simulation results of their electrical conductivities and Seebeck coefficients. As seen in Fig. 7, although the Seebeck coefficient of the non-planar barrier is lower, its total *ZT* is higher than that of the planar barrier due to its largely increased electrical conductivity. It is shown that the *ZT* enhancement decreases with the increase of the reduced Fermi energy in the range of interest.

In conclusion, nonplanar heterostructure potential barriers improve upon their planar counterparts by increasing the number of electrons thermally emitted, as evidenced by the Monte Carlo simulations. The current enhancement increases with the potential barrier height, and depends on the geometry of the interface microstructure. We have shown that the thermoelectric figure of merit *ZT* can also be improved by using a nonplanar barrier.

[1]G. S. Nolas, J. Sharp, and H. J. Goldsmid, *Thermoelectrics: Basic Principles and New Materials Developments* (Springer, Berlin, 2001).
[2]A. Shakouri and J. Bowers, Appl. Phys. Lett. **71**, 1234 (1997).
[3]G. D. Mahan and L. M. Woods, Phys. Rev. Lett. **80**, 4016 (1998).
[4]M. D. Ulrich, P. A. Barnes, and C. B. Vining, J. Appl. Phys. **90**, 1625 (2001).
[5]G. Chen and A. Shakouri, ASME J. Heat Transfer **124**, 242 (2002).
[6]S. T. Huxtable, A. R. Abramson, C. L. Tien, A. Majumder, C. Labounty, X. Fan, G. Zeng, J. E. Bowers, A. Shakouri, and E. T. Croke, Appl. Phys. Lett. **80**, 1737 (2002).
[7]D. Vashaee and A. Shakouri, Phys. Rev. Lett. **92**, 106103 (2004).
[8]D. L. Smith, E. Y. Lee, and V. Narayanamurti, Phys. Rev. Lett. **80**, 2433 (1998).
[9]M. Kozhevnikov, V. Narayanamurti, C. Zheng, Y. J. Chiu, and D. L. Smith, Phys. Rev. Lett. **82**, 3677 (1999).
[10]B. Moyzhes and V. Nemchinsky, Appl. Phys. Lett. **73**, 1895 (1998).
[11]B. L. Ward, O.-H. Nam, J. D. Hartman, S. L. English, B. L. McCarson, R. Schlesser, Z. Sitar, R. F. Davis, and R. J. Nemanich, J. Appl. Phys. **84**, 5238 (1998).