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Electrical and thermal characteristics of multilayer thermionic power devices

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Abstract—Electron thermal transport in semiconductor thermionic devices is investigated numerically. The efficiency of thermionic devices is dramatically reduced by the conduction heat current, $\Delta T/R^{th}$. One approach to reduce the thermal conductivity is to use layered structures where interface scattering can increase the thermal resistivity. It is found that the temperature gradient across the devices can be increased by a factor of 2 in the presence of phonon scattering. The device is more efficient at elevated temperature.

I. INTRODUCTION

Solid-state power devices have attracted much attention in recent years due to their reliability, compatibility, and reduced environmental impact [1], [2], [3]. One class of such devices is based on thermionic emission in semiconductor-semiconductor or metal-semiconductor multilayers. The main challenges in designing a practical thermionic device are to maximise the thermal emission of electrons and to minimise the heat back-flow due to phonons. Mahan *et al.* [4] proposed using a multi-barrier system, reasoning that using N barriers identical to a single barrier would reduce the temperature gradient across each barrier to $\sim \Delta T/N$, effectively reducing the back-flow by a factor of N . A second advantage of using a multi-barrier system stems from experimental work carried out on the thermal conduction of superlattices as compared to bulk materials [5]. Following this experimental work, theoretical work was carried out to explain the reduced thermal conductivity of superlattices as compared to bulk materials. By solving the Boltzmann Transport Equation for phonons and using various phonon interface scattering mechanisms, Chen [6] successfully modelled the majority of these experimental results. The theoretical results presented show that the thermal conductivity of superlattices is roughly proportional to the square root of the thickness of each of the layers. If the total width of the a superlattice is held constant this is equivalent to saying that, for a fixed sample size, the thermal conductivity decreases proportionally to the number of barriers in the sample. This paper will investigate this concept in detail and show that increased heat power removal is possible with a multi-barrier system. We will investigate the maximum cooling for 10-barrier structures using different materials.

II. MODELS AND METHODS

We consider a number of single-barrier devices sandwiched together as shown in Fig. 1. In general the potential on the left of a barrier, ϕ_i^L , may or may not be larger than the potential

to the right, ϕ_i^R . By restricting the discussion to devices where $\phi_i^L \geq \phi_i^R$, we can ignore ϕ_i^R altogether and use:

$$\phi_i^L \rightarrow \phi_i \quad (1)$$

Dealing with such a system analytically becomes cumbersome, although it can be done quite effectively [7]. One approach to solving the system of equations is to use numerical methods. This has a number of distinct advantages such as new physics being easily included into the model and the ability to read out any device parameters once convergence has been reached. In addition to this, solving the system under different conditions becomes straightforward once the basic system has been developed. For instance, determining the bias at which a given device operates with maximum power output is easily found by solving the equations whilst varying the applied bias in the direction that increases the power output. Here we shall develop a numerical method to directly calculate the electrical and heat current.

Fig. 1. Multilayer Thermionic Devices

Fig. 1 shows the multilayer thermionic cooler that is to be simulated. The width of each barrier is less than the carrier mean-free path and greater than the tunnelling width. Electrical and thermal continuity must be ensured at each electrode. To do so involves solving a number of simultaneous equations which are detailed below. In the following sections, net electrical and energy currents are assumed to be positive when moving from left to right.

A. The electrical and heat current

The net electrical current across the i^{th} barrier is given by [8],

$$J = J_i = AT_{i-1}^2 \exp\left(\frac{-q\phi_{i-1}}{k_B T_{i-1}}\right) - AT_i^2 \exp\left[\frac{-q(\phi_{i-1} + V_i)}{k_B T_i}\right] \quad i = 1, 2, \dots, N \quad (2)$$

It should be noted that this current is constant throughout the device. Assuming net heat current flow is from left to right, the energy current leaving the i^{th} electrode to the right is given as [8],

$$J_{qi}^{out} = \left(\phi_i + \frac{2k_B T_i}{q} \right) AT_i^2 \exp\left(\frac{-q\phi_i}{k_B T_i}\right) - \left(\phi_i + \frac{2k_B T_{i+1}}{q} \right) AT_{i+1}^2 \exp\left(\frac{-q(\phi_i + V_{i+1})}{k_B T_{i+1}}\right) - \frac{T_{i+1} - T_i}{R_{i+1}^{th}(N)} \quad i = 1, 2, \dots, N \quad (3)$$

and the energy current entering the i^{th} electrode from the left is given by,

$$J_{qi}^{in} = \left(\phi_{i-1} + V_i + \frac{2k_B T_{i-1}}{q} \right) AT_{i-1}^2 \exp\left(\frac{-q\phi_{i-1}}{k_B T_{i-1}}\right) - \left(\phi_{i-1} + V_i + \frac{2k_B T_i}{q} \right) AT_i^2 \exp\left(\frac{-q(\phi_{i-1} + V_i)}{k_B T_i}\right) - \frac{T_i - T_{i-1}}{R_i^{th}(N)} \quad i = 1, 2, \dots, N \quad (4)$$

where $R_i^{th}(N)$ is the thermal resistivity of the i^{th} barrier for an N -barrier system. If increased thermal resistance due to interface scattering or superlattices is considered, in general $R_i^{th}(N) \neq R_i^{th}(N-1)$.

For continuity of heat current, $J_{qi}^{in} = J_{qi}^{out}$. Note, $J_{qi}^{in} - J_{q(i-1)}^{out} = V_i J \neq 0$, where $V_i J$ is the work needed to produce cooling across the i^{th} barrier. For continuity of electrical currents $J_{i-1} = J_i = J_{i+1} \dots$. In this device configuration there are N barriers — numbered 1 to N ; and $(N+1)$ electrodes — numbered 0 to N . The first $(N-1)$ variables in the vector, $\mathbf{x}$, are the biases across each barrier (or the bias of electrode i with respect to the bias of electrode $i-1$). The bias across the last barrier is set and so is not an unknown. The second $(N-1)$ variables are the temperatures of each electrode numbered 1 to $N-1$. The temperature of the 0th and N^{th} barriers are set and so are not unknowns. The first $(N-1)$ equations are the electrical currents entering each electrode from the left minus the current exiting to the right. The second $(N-1)$ equations are the energy currents entering each electrode from the left minus that exiting to the right. For convergence, these equations should equal zero. A net electrical and heat current is assumed to flow from left to right in the device. In order to ensure continuity of electrical and heat currents through the device, these $2(N-1)$ equations must be solved simultaneously; i.e., the variables are varied until each equation satisfies the following criteria:

$$|F_i| \leq \text{Tol}, \quad i = 1, 2, 3, \dots, 2(N-1) \quad (5)$$

where $F_i = J_{i-1} - J_i$ for $0 < i \leq N$ or $F_i = J_{q,i-1} - J_{q,i}$ for $N < i \leq 2N$, and Tol is the tolerance of the search.

B. Parameters and Boundary Conditions

The barrier height and thermal resistance of each node can be set and are considered parameters of the system. The bias across the last barrier V_N and temperature of the first and last

Fig. 2. Minimum Cold Electrode Temperature vs. Applied Bias : $i = 0$ 1 V $h = 300$ K $t_i^{th} = 41.14 \times 10^{-9}$ m²·K/W $\ast = 1$ = 1 10.

electrodes (T_0 and T_N) are set. All of the other biases and temperatures of the system are varied using Newton's Method until the continuity equations are solved. Once the system has converged the total bias across the device can be calculated. In fact, once convergence has been reached the real advantages of a numerical system become apparent as any variable of the system can be read out in order to readily achieve such results as temperature and bias profiles across the system.

III. EFFICIENCY OF MULTI-BARRIER DEVICES

Once the equations have been solved for a given set of parameters (such as work function and barrier thickness), the efficiency of each device is calculated in order to compare the performance of different systems. The efficiency of the device is the heat taken from the cold side divided by the work needed to do so and is given by $\eta = \frac{J_{qc}}{J_c V}$ where $V = \sum_{i=1}^N V_i$.

The motivation for moving from a single- to multi-barrier system was to overcome decreasing device efficiency due to heat conduction and to ensure that the devices are operating thermionically (i.e., electrons move ballistically across each barrier). It was proposed that having a number of barriers would decrease ΔT across each barrier and so heat conduction would be reduced at each layer. Simulation results have shown that while ΔT is reduced at each barrier, the overall efficiency of the device does not increase as the number of barriers increases. By slightly modifying the model used (making R dependent on N) it is shown that the multi-barrier system may be more efficient than a single-barrier system.

As an alternative to decreasing ΔT across each barrier, the conduction heat current can be decreased by increasing the effective thermal resistivity, R , across each barrier. Thus, the multi-layer cooler may turn out to be more efficient for reasons different to those proposed.

Consider just the first two electrodes of a multi-barrier device. When a bias is initially applied a heat current due to thermionic emission will leave the first and enter the second electrode. This will cause the first electrode to cool and the

second to heat. This will increase the temperature gradient across the first barrier and thus the backward heat flow due to conduction will also increase. This will, in turn, increase the temperature of the first electrode and decrease the temperature of second electrode. This reduces both the net heat current due to thermionic emission and the heat current due to conduction. This process will continue until the net heat current leaving the cold electrode equilibrates.

The cold temperature of the device can be varied at a set applied bias to find when the net heat current leaving the cold electrode is zero. This is achieved by using a Newton-Raphson scheme in 1-dimension with T_c now the variable and V_N held constant. By doing this for a range of biases the cold-electrode temperature dependence on applied bias can be found.

Fig. 2 shows variation of cold electrode minimum temperature with applied bias for a device with $\phi_i = 0.1$ V, $R_{th} = 41.14 \times 10^{-9}$ m²K/W. Both a single- and 10-barrier device results are shown. The multiple-barrier device can achieve a much lower cold-electrode temperature.

As is expected, a negative applied bias increases the heat flow from hot- to cold- electrode and thus causes an increase in the cold-electrode temperature. A positive applied bias initially causes the cold electrode of the devices to decrease as heat is removed. For the single barrier device this temperature plateaus as the heat current removed from the cold side saturates. For the 10-barrier device a global minimum cold electrode temperature is achieved at an applied bias of around 0.14 V. As the applied bias is further increased the temperature begins to increase again due to the heat current decreasing.

TABLE I
CALCULATED MATERIAL PARAMETERS

Material	(nm)	Max. R^{th}
GaAs (n)	81.8	1.49
GaAs (p)	11.0	0.20
Al _{0.07} Ga _{0.93} As (n)	72.0	1.74
InSb (n)	349.3	19.42
InSb (p)	21.4	1.19
InP (n)	58.6	0.861
InAs (p)	232.6	8.615
Ga _{0.47} In _{0.53} As (n)	93.2	18.63

The performance of a thermionic device is crucially dependent on two materials parameters, which are listed in Table I: the mean-free path (λ) and maximum thermal resistance per unit area (in units of 10^{-9} K·m²/W). Here (n) and (p) refer to electrons and holes being majority carriers, respectively. This can be achieved by either doping the material with donors or acceptors, or by surrounding the barrier material with highly doped regions.

From Table I it may be seen that n-type InSb and n-type Ga_{0.47}In_{0.53}As have much higher maximum thermal resistance per unit area than the other materials. n-type InSb, though, has a comparatively low effective mass. A reduced thermal mass means that, on average, less energy is transported per electron contributing to thermionic current. It might be mentioned that n-type Ga_{0.47}In_{0.53}As has a larger effective mass, although it

is not as large as for materials where holes are the majority carriers. These two materials will be of interest for use in devices. It should be noted that Ga_{0.47}In_{0.53}As has a much larger thermal resistivity than that of the related binaries (InAs and GaAs). This can be attributed to lattice disorder due to the random distribution of constituent atoms in the two sublattice sites.

With its relatively large effective mass, mobility and thermal resistivity, we focus on n-type Ga_{0.47}In_{0.53}As. Comparing with n-type InSb, it has a much larger thermal resistivity, but due to its increased effective mass and reduced mobility (and therefore reduced mean-free path), the maximum thermal resistance per unit area for Ga_{0.47}In_{0.53}As is slightly less than InSb, although still much larger than the other materials.

The effective mass and thermal resistance of materials are two important parameters that affect device performance. Due to the effective mass appearing in the expression for mobility, and therefore mean-free path and maximum thermal resistance per unit area, a numerical solution is used to compare different materials. Fig. 3 shows the maximum cooling for 10-barrier structures operating with the hot electrode at 300 K. By trying different barrier heights it was found that the cooling power increases substantially with decreasing barrier height (the same is not necessarily true for efficiency). A barrier height of 77 meV is used for the devices. This value is the minimum value for which Maxwell-Boltzmann statistics are still valid in the model.

By trying different numbers of barriers it was found that there is substantial increase in device performance between 1- and 10- barrier systems. Increasing the number of barriers further, to say 20 or 50, does not substantially increase the performance of the devices, but does add to the complexity of their fabrication.

TABLE II
MAXIMUM COOLING FOR DIFFERENT MATERIALS - *: INCREASED THERMAL RESISTIVITY DUE TO PHONON SCATTERING

Material	Δ_{max} (K)	Δ_{max}^* (K)
GaAs (n)	0.135	0.426
Al _{0.07} Ga _{0.93} As (n)	0.182	0.573
InSb (n)	0.413	1.289
InP (n)	0.105	0.331
Ga _{0.47} In _{0.53} As (n)	1.147	3.511

Table II summarises the results for selected materials deduced from Fig. 3. The second column shows the maximum cooling possible for a 10-barrier structure made of the material in column one, operating at a temperature of 300 K with a barrier height of 77 meV. The third column shows the maximum cooling for the same material, but with the thermal resistivity of the material increased due to phonon scattering. This mechanism is approximated by multiplying the bulk resistivity by the square root of the number of barriers. This is done in accordance with the increase in thermal resistivity of superlattices modelled by Chen [6].

The devices used earlier are GaAs/AlGaAs based systems. The Al concentration is around 7% in the heterostructure

barriers. The maximum cooling for a 10-barrier system is expected to be around 0.18 K if bulk thermal resistivity is used and 0.57 K if an increase in phonon scattering is assumed. Because the barriers are made from GaAs, the maximum cooling is expected to lie between the value for the two different values i.e. between 0.14 and 0.18 K if bulk resistivity is used or 0.43 and 0.57 K if increased thermal resistivity is assumed.

IV. CONCLUSIONS

The advantages of using a multiple-barrier system were confirmed by the fact that considerably more cooling power is achievable whilst only having a slight loss in device efficiency. By having only around $\Delta T/N$ temperature drop across each barrier (as opposed to ΔT for a single-barrier system) more heat is removed from the cold side of the device due to reduced heat conduction across each barrier. In addition to this, further heat is removed when phonon scattering due to interfaces between materials is taken into account. This results in greater cooling than for single-barrier devices.

Due to the work done in transporting carriers across each barrier it was found that the heat transport increases throughout the device. In some cases this increases the temperature of intermediate electrodes above the temperature of both the end electrodes. This may appear to be a waste of energy, but multi-barrier systems still out perform single-barrier systems. If this heat could be removed by some other means (such as optical emission) the performance of the devices would be increased further.

By employing a numerical solution to the problem many advantages of such a system become apparent. Once convergence of the system equations has been reached, the performance of devices can be modelled under a multitude of different conditions. For instance, the maximum cooling for a given applied bias can be found by varying the temperature of the cold side until the heat current leaving the first electrode is zero. Likewise, the maximum cooling for a combination of device parameters can be found by repeating this step for a range of applied biases until the minimum cold temperature is achieved.

It is found that these devices operate more efficiently at elevated temperatures due to the increased average energy of carriers. This means that these devices may have applications at high temperature, such as running the devices in reverse as power generators.

Increased effective mass generally means increased cooling power and efficiency, due to the effective mass of carriers appearing in the numerator of Richardson's constant. But the effective mass also appears in the equation for mean-free path of carriers, which in turn sets the maximum thermal resistance per unit area possible for different materials. Because of the complex interplay between effective mass and maximum thermal resistance, graphical methods were used to compare the theoretical minimum temperature for 10-barrier devices. For the devices modelled here, cooling of less than half a degree is expected.

Fig. 3. Maximum Cooling of Cold Electrode vs. Device Parameters.
 $i = 77$ meV $\mu = 300$ K $N = 10$.

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REFERENCES

- [1] C. J. LaBounty, A. Shakouri, P. Abraham, and J. E. Bowers, Proc. SPIE, **3950**, 69 (2000).
- [2] L. Rushing, A. Shakouri, P. Abraham, and J. E. Bowers, Proc. 16th Int. Conf. Thermoelectrics, IEEE, 646 (1997).
- [3] A. Shakouri, C. LaBounty, J. Piprek, P. Abraham, and J. E. Bowers, Appl. Phys. Lett. **74**, 88 (1999).
- [4] G. D. Mahan, J. O. Sofo, and M. Bartkowiak, J. Appl. Phys. **83**, 4683 (1998).
- [5] S.-M. Lee, D. G. Cahill, and R. Venkatasubramanian, Appl. Phys. Lett. **70**, 2957, (1997).
- [6] G. Chen, Phys. Rev. B **57**, 14958 (1998).
- [7] G. D. Mahan and L. M. Woods, Phys. Rev. Lett. **80**, 4016 (1998).
- [8] B. Lough, S. P. Lee, R. A. Lewis, and C. Zhang, Computer Phys. Commun. **142**, 274 (2001).