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Thermal characteristics of a microscopic model of thermal transistor

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ABSTRACT

We study an in-depth operation of a microscopic model of thermal transistor consisting of Fermi – Pasta – Ulam – β like lattices. The output and the transfer characteristics of thermal transistor have been reported, which are very analogous to its counterpart characteristics of an n-channel FET. Here, we coined and identified terminology like thermal Fourier region, thermal knee point, thermal pinch-off point and thermal saturation region from output characteristics of thermal transistor. Thermal source resistance, thermal transconductance and thermal amplification factor have been defined and computed for different gate temperatures. Our non-equilibrium molecular dynamics simulation study shows an amplification of output thermal current ≈ 218 times with thermal transconductance 0.0164 ± 0.0007. First ever equation for output thermal current $J_S = J_{SS}\left[1 - \frac{T_{GS}}{T_P}\right]^2$ is numerically established which is very analogous to that of Shockley's equation for FET.

1. Introduction

It is known that the electric current and heat current are vital in the transport of energy. About 90% of energy consumption of the world is through heat, but efforts in controlling the flow of heat are not exhaustive [1]. Heat, a source of such form of energy is lattice vibrations usually treated as unwanted energy and believe to deteriorate the efficiency of semiconductor devices. A lack of excitement for studying the heat conduction in low dimensional system observed in the past is due to less advancement in technology perspective compared with its electronic equivalent current conduction and hence, there does not exists the device that can manage and harvest the heat energy [2–4]. There is only one type of heat carrier 'phonon', obeys Bose-Einstein statistics. Hence, asymmetric phononic flow through materials not expected unless there exist an orientation of applied temperature gradient or asymmetric mass distribution along the space. As phonons are quasi-particles without bare charge and bare mass, it is a challenge for the scientists to find out proper mechanism by which the flow of phonons can be controlled efficiently at nano scale. Now, the significant interest toward the study of heat conduction in nanoscale materials been increased and enriched the underlying mechanism of phonon transport both at theory and at experiment [5–8]. At room temperature, the wavelength of 1–3 nm and mean free path of 10–100 nm are the two characteristics lengths available to heat carrying phonons in solids. Hence, researchers and engineers can use nanostructures of this length scale in the process of heat management [5,9]. Scientific outcome of these studies are very much important in energy transport through heat in nano-tube, nano-wire, nano-horn, nano-cone, nano-ribbons, nano-channels and nano-roads [10–23]. Such outcome have opened the possibility of realizing thermal devices like thermal rectifier, thermal diode, thermal transistor, thermal logic gates, thermal memory, acoustic diode, revere diode; and functional graded materials, quantum structures and networks as a potential structure for guiding the heat transport [24–42].

Based on the progress made to study thermal transport at nanoscale [23,43,44], now we know that if thermal transistor is fabricated successfully and it practiced, it will be one of the fundamental building block of thermal circuits, which may governs the operation of various phononic devices in future. In spite of this, rigorous attempts of modeling thermal transistor are not found in the literature. In Li et al.'s [29,30,45] model of a thermal transistor, the phenomena of negative differential thermal resistance is used. They shown through numerical simulation that the model can work as a heat switch and heat modulator under certain simulation parameters. By electronic analogy, one may inspire in designing

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similar thermal devices that could control heat current. However, in realization of gate controlled three terminal thermal devices, only amplification effect is studied in depth [29,30,45]. Not a single attempt found for studying the characteristics of a thermal transistor, which are very analogous to Field Effect Transistor (FET), its electronic counter part [46]. Like FET, in thermal transistor, the phonons play an important role in thermal transport makes it unipolar thermal device. Negative voltage on gate terminal controls the width of channel in FET. Similar to FET, the negative temperature gradient on gate terminal controls the width (not physical) of the phonon channel [34]. The thermal current within drain and source is control excellently on applying the small temperature at gate terminal. Inspired by this electrical analogy with FET and the technological importance of nanoscale thermal transport, a microscopic model of a thermal transistor is proposed and first ever in-depth study on the characteristics of a thermal transistor are reported in the present paper.

2. Model and methodology

In the study of thermal transport at low dimension, among the various available lattice models [2,3], Fermi-Pasta-Ulam (FPU) model [47] remains the first choice of researcher for explaining the interatomic interaction. The FPU model has two special cases with cubic nonlinearity and quartic nonlinearity referred as FPU-α and FPU-β models respectively [47]. FPU − α model alone is not suitable for non-equilibrium molecular dynamics simulation, because the system is not stable due to the cubic nonlinear potential, which causes the particles to escape to infinity and thus bound states cannot exist at all in such a potential whereas FPU − β model has stable trajectories. Hence, we used the FPU-β model to write the Hamiltonian as,

$$H = \sum_{i=1}^{N}\left[\frac{p_i^2}{2m} + \frac{k}{2}(x_i - x_{i-1})^2 + \frac{\beta}{4}(x_i - x_{i-1})^4\right] \quad (1)$$

Our system of choice for constructing one − dimensional (1D) microscopic model of thermal transistor is consisting of three FPU-β lattices [47] referred as Source (S), Drain (D), and Gate (G). One end of each lattice is connected to a junction particle (O) via harmonic potential and second ends with heat reservoir, as in Fig. 1.

The Hamiltonian of above *1D* anharmonic lattice structure consisting of Source (S), Drain (D), and Gate (G) connected to an interfacial junction particle O, written as [29,30,45],

$$H = H_S + H_D + H_G + H_{\text{int}} \quad (2)$$

$$\begin{aligned} H = {} & \sum_{i=1}^{N_S}\left[\frac{p_{S,i}^2}{2m_S} + \frac{k_S}{2}(x_{S,i} - x_{S,i-1})^2 + \frac{\beta}{4}(x_{S,i} - x_{S,i-1})^4\right] + \sum_{i=1}^{N_D}\left[\frac{p_{D,i}^2}{2m_D}\right. \\ & \left. + \frac{k_D}{2}(x_{D,i} - x_{D,i-1})^2 + \frac{\beta}{4}(x_{D,i} - x_{D,i-1})^4\right] + \sum_{i=1}^{N_G}\left[\frac{p_{G,i}^2}{2m_G}\right. \\ & \left. + \frac{k_G}{2}(x_{G,i} - x_{G,i-1})^2 + \frac{\beta}{4}(x_{G,i} - x_{G,i-1})^4\right] + \frac{p_O^2}{2m_O} \\ & + \frac{k_{\text{int}S}}{2}(x_{N_S} - x_O)^2 + \frac{k_{\text{int}D}}{2}(x_{N_D} - x_O)^2 + \frac{k_{\text{int}G}}{2}(x_{N_G} - x_O)^2 \end{aligned} \quad (3)$$

Here N_S, N_D, and N_G are the number of oscillators for source, drain and gate segments, $x_{S,i} - x_{S,i-1}$, $x_{D,i} - x_{D,i-1}$, and $x_{G,i} - x_{G,i-1}$ are particle displacement from their equilibrium positions. $x_{N_S} - x_O$, $x_{N_D} - x_O$ and $x_{N_G} - x_O$ are particle displacements of the last particle of respective segments *S*, *D*, and *G* from its equilibrium position with respect to the interface particle *O*. $p_{S,i}$, $p_{D,i}$, $p_{G,i}$ and p_O are linear momentum and $m_{D,S,G,O}$ is the mass of an oscillator in respective segments. β is anharmonicity parameter of FPU- β model. k_S, k_D, k_G, k_{intS}, k_{intD} and k_{intG} are appropriate spring constants. In our numerical simulation, Nosé − Hoover [48,49] deterministic heat baths are applied to the first particle of each segment to maintain the temperature gradient along each segment. Fix boundary condition is used for the present work by considering $x_{S,0} = x_{D,0} = x_{G,0} = 0$.

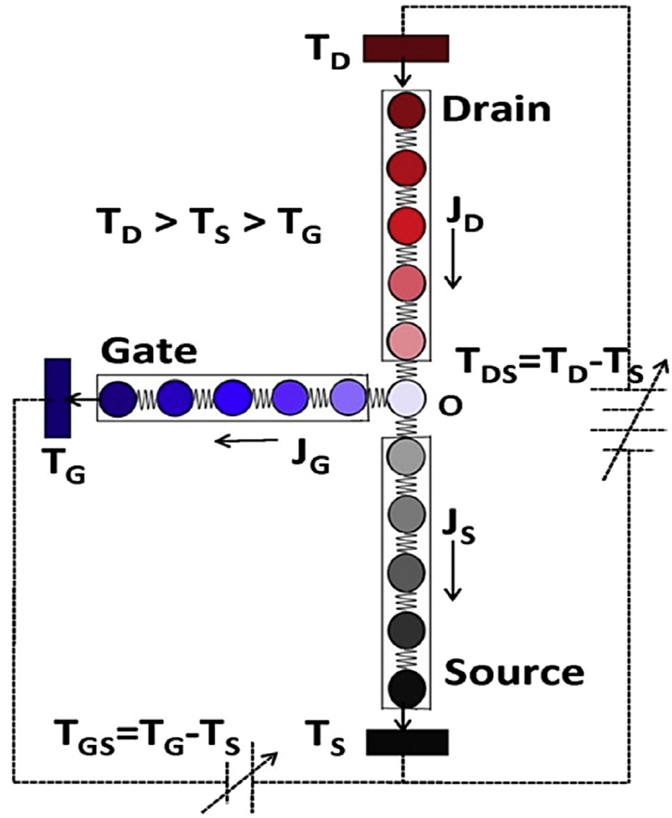

Fig. 1. Schematic representation of *1D* microscopic model of thermal transistor. J_S, J_D and J_G are the heat currents flowing through Source (S), Drain (D) and Gate (G) terminals, respectively. T_S, T_D and T_G are the temperature of heat baths connected to Source (S), Drain (D) and Gate (G) terminals, respectively. T_{DS} and T_{GS} represent the temperature of Drain and Gate terminal with respect to Source temperature (or temperature difference between respective segments).

The equations of motion of the particles then have the following form,

$$m_{S,D,G,i}\ddot{x}_{S,D,G,i} = F_{S,D,G,i} - F_{S,D,G,i+1} - \zeta_{S,D,G,1}\dot{x}_{S,D,G,1}\delta_{i,1} \quad (4)$$

With the equations of motion of the particles connected with junction particle are,

$$m_{S,D,G}\ddot{x}_{N_{S,D,G}} = F_{N_{S,D,G}} - F_O \quad (5)$$

and

$$\dot{\zeta}_{S,D,G} = \frac{\dot{x}_{S,D,G,1}^2}{T_{S,D,G}} - 1 \quad (6)$$

Here $F_i = -\partial H/\partial x_i$ is the force on i^{th} oscillator. The $T_{S,D,G}$ is the temperatures of attached heat baths. $\zeta_{S,D,G}$ is the Nosé-Hoover thermostat parameter and implements the microscopic interaction of the first particle with the heat reservoir [2,3,48,49]. When the temperature of the particles in S, D or G increases than T_S, T_D or T_G,