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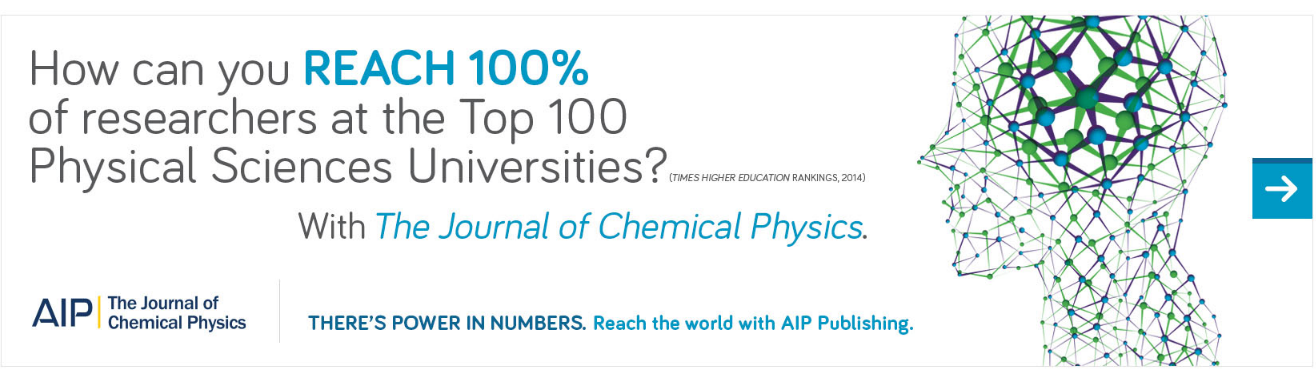

Communication: A tractable design for a thermal transistor

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We propose a conceptual design for a logic device that is the thermal analog of a transistor. It has fixed hot (emitter) and cold (collector) temperatures, and a gate controls the heat current. Thermal logic could be applied for thermal digital computing, enhance energy conservation, facilitate thermal rheostats, and enable the transport of phononic data. We demonstrate such a device using molecular dynamics simulations that consider thermal transport across hot and cold solid Si regions that seal water within them. Changes in the hot side, or emitter, heat current are linear with respect to varying gate temperature but the corresponding variation in the collector current is nonlinear. This nonlinear variation in collector current defines the ON and OFF states of the device. In its OFF state, the thermal conductivity of the device is positive. In the ON state, however, more heat is extracted through the cold terminal than is provided at the hot terminal due to the intervention of the base terminal. This makes it possible to alter the transport factor by varying the gate conditions. When the device is ON, the transport factor is greater than unity, i.e., more heat is rejected at the collector than is supplied to the emitter. © *2013 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4826316]

We present a unique conceptual design of a logic device that is the thermal analog of a transistor.[1] Since structural manipulations of inhomogeneous solids are typically more energy intensive (and often impossible) than available pathways to change the nature of solid-liquid interfaces,[2–6] our design is based upon solid-fluid resistances. It has fixed hot (emitter) and cold (collector) temperatures. A gate controls the heat current and thus temperature just as its electronic counterpart controls the electric current or voltage in a conventional transistor. The hot reservoir of such a three-terminal thermal transistor serves as the emitter H, the cold reservoir as the collector C, and smaller input reservoirs collectively behave as the base G. The associated heat fluxes, or currents, in such a transistor are Q_H, Q_C, and Q_G, respectively.

Changing the base temperature T_G alters the transport factor $\alpha = |Q_C/Q_H|$, which represents the ratio of the collector to the emitter heat currents, and the flux gain $\beta = -Q_C/Q_G$ that compares the collector and base heat currents. If α and β are varied by changing T_G but without altering the driving potential of the system, which is the overall temperature difference $(T_H - T_C)$ across the emitter and collector, the resulting control over the thermal transport enables thermal logic.

The use of thermal gates should provide significant savings in power consumption since, in many cases, accessible thermal energy in the form of waste heat would be used. Conceivably, thermal logic could be applied for thermal digital computing, e.g., a computer that uses waste heat rather than electricity to operate, or to enhance energy conservation.[1–5] It could facilitate the development of thermal rheostats or enable the transport of phononic data using high frequency (GHz) thermal currents. The resulting devices could be used in solar energy collectors, heat pumps, and internal combustion engines.[1–5]

The utility of solid-liquid interfaces for thermal logic arises from their variable surface wettability. When the wettability is altered, so is the solid-fluid interfacial thermal resistance, which leads to variable thermal transport that enables thermal rectification and thermal transistors.[1,6,7] Since the dynamics that influence the solid-fluid interfacial thermal resistance are nonlinear,[6–10] their use leads to tunable thermal devices. At the nanoscale, the manipulation of phonon transport,[1,2] e.g., through solid-solid or solid-fluid mass reorganization,[10–14] to enable thermal logic is straightforward.[1,2,4] Here, we present a tractable design for a thermal transistor by exploiting solid-fluid interfaces, which, being versatile, can be readily manipulated to become more hydrophobic or hydrophilic.[7–10]

Consider the heat current Q due to a thermal potential, or temperature difference, ΔT that must overcome a system resistance $R = \Delta T/Q > 0$. To design the thermal analog of a semiconductor device, the resistance must be manipulated so that Q decreases with increasing ΔT.[2,5,15] When ΔT is specified, another input or output, such as through a base terminal in a three terminal electronic transistor,[1] can be used to vary R. Thus, the current across the other two terminals can be manipulated in a nonlinear manner. The design of the practical thermal logic device, shown in Fig. 1, constrains a fluid in a sealed nanoscale reservoir. Designated sections of the two opposing solid walls of the cuboid that are of ∼1 nm thickness are maintained at T_H and T_C while designated sections of the other two walls are constrained at the base temperature T_G, as shown in Fig. 1(b). This arrangement creates a synergy between the three thermal resistances, R_H, R_C, and R_G which regulate the currents Q_H, Q_C, and Q_G, respectively. From energy conservation, $Q_H + Q_G = Q_C$.

The molecular dynamics (MD) simulations used to demonstrate the feasibility of such a device considers thermal transport across hot and cold solid regions that enclose

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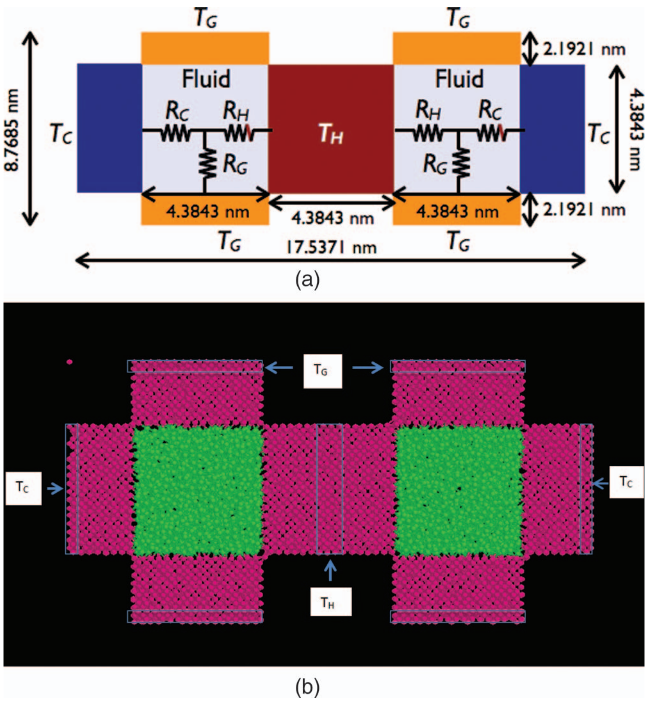

FIG. 1. (a) The thermal logic device couples constrain a fluid in a nanoscale reservoir. Two opposing walls of the cuboid are at hot and cold temperatures, T_H and T_C, while the other two walls are at the base temperature T_G. This produces three thermal resistances, R_H, R_C, and R_G, which regulate the currents Q_H, Q_C, and Q_G. (b) MD simulation setup where the solid walls are a silicon crystal with Si atoms as red spheres and water, shown by green spheres, has a density $\rho \sim 980$ kg/m^3. The system consists of 2818 molecules of H_2O and 8220 atoms of Si.

a sealed fluid, as shown in Fig. 1. The solid walls have the structure of a silicon crystal, where Si is represented by red spheres, while the fluid, which is water shown by green spheres, has a density $\rho \sim 980$ kg/m^3. The system consists of 2818 molecules of H_2O and 8220 atoms of Si. All Si atoms are tethered/attached to their equilibrium sites and allowed to vibrate harmonically. The system is ∼17.54 nm long and 8.77 nm wide with a depth (in the plane of Fig. 1) of ∼2.19 nm. Periodic boundary conditions are applied in all three directions.

The molecules simulated have Gaussian velocity distributions initially. The controlled hot and cold solid regions in Fig. 1 are imparted average temperatures $T_H = 1209$ K and $T_C = 403$ K with a Gaussian thermostat, while the controlled temperature T_G of the gate regions is varied between 403 and 1209 K. A Gaussian thermostat is used as it found to be efficient for nonequilibrium studies. Its linear response in the thermodynamic limit is also identical to that of the Nose-Hoover thermostat.[16,17] This leads to a globally averaged fluid temperature $(T_H + T_C)/2 \sim 806$ K with slight variations depending upon T_G. At these temperatures the bulk fluid are supercritical. These higher wall temperatures facilitate larger heat transfer rates and minimize data scatter. We emphasize that the fundamental aspects of nanoscale thermal transport that apply at lower temperatures remain unaltered.[6,7] The (N,V,T) simulations use step sizes of 1 fs. Results are reported after the simulations have completed 2×10^6 time steps or more and approach steady state. We have also carried out longer simulations to confirm the accuracy and stability of the temperature and density profiles.

The MD algorithm utilizes the quaternion method.[1,6,7] Intermolecular interactions are based on the potential model $u_{ij} = 4\varepsilon_{ij}((\sigma_{ij}/r_{ij})^{12} - (\sigma_{ij}/r_{ij})^6) + (Q_iQ_j)/r_{ij}$, where σ_{ij} and ε_{ij} represent the L-J parameters. For water, the model has two H-atom sites and one O-atom site, r_{ij} is the scalar distance between sites i and j, and Q_i and Q_j are the charges on these sites. The SPC (simple point charge potential) potential which realistically represents water properties, including its thermal conductivity as a supercritical fluid[18] is used. Si is modeled with an L-J potential. Additional details of the method are described in a previous publication.[1] There, we introduced a design for a thermal logic device that manipulated the solid-liquid interfacial thermal resistance by varying the surface wettability from hydrophobic to hydrophilic.

The response of the device to varying base temperature is presented in Fig. 2. Each dimensionless unit of T corresponds to 806 K. When T_G is held at the average system temperature of unity, the base current $Q_G \approx 0$, where each dimensionless unit of Q corresponds to 4.26 μW. This current is negative when $T_G < 1$, i.e., Q_G is an outward heat flux from the system. It is positive when $T_G > 1$, i.e., Q_G is an inward flux. The variation of Q_G with changing T_G is nonlinear. However, since changes in the hot side, or emitter, current Q_H are linear with respect to varying T_G, the corresponding variation in Q_C is nonlinear.

At a simple level, the nonlinear variation in the collector current defines the ON and OFF states of the device. When Q_C is outward and small (and roughly constant), the device may be considered to be OFF. In this state, most of the outward current from the device is routed through the base. When the outward current shifts exclusively to the collector, i.e., the base now becomes a source of inward current, the device may be considered to be ON. In other words, when $Q_C < Q_G$ and $Q_G < 0$, the device is OFF whereas it is ON when $Q_C < 0$ and $Q_G > 0$.

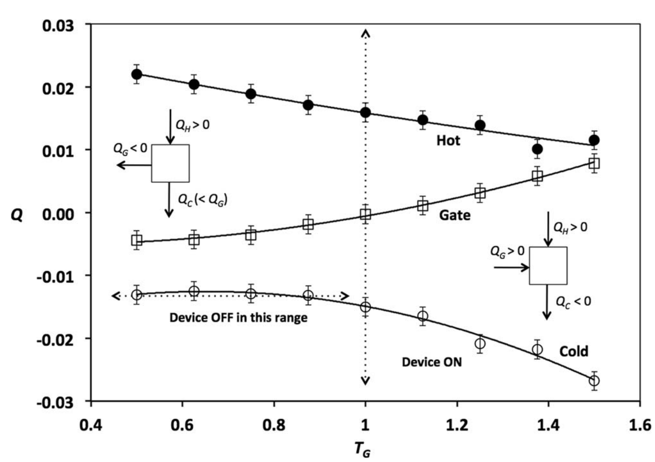

FIG. 2. The variations in the hot (emitter), cold (collector), and base heat currents Q_H, Q_C, and Q_G with changing base temperature T_G. The nonlinear variation in Q_C defines the ON and OFF states of the device. When $Q_C < Q_G$ and $Q_G < 0$, the device is OFF whereas when $Q_C < 0$ and $Q_G > 0$, it is ON. Each dimensionless unit of temperature corresponds to 806 K, while each corresponding unit of Q is equivalent to 4.26 μW.

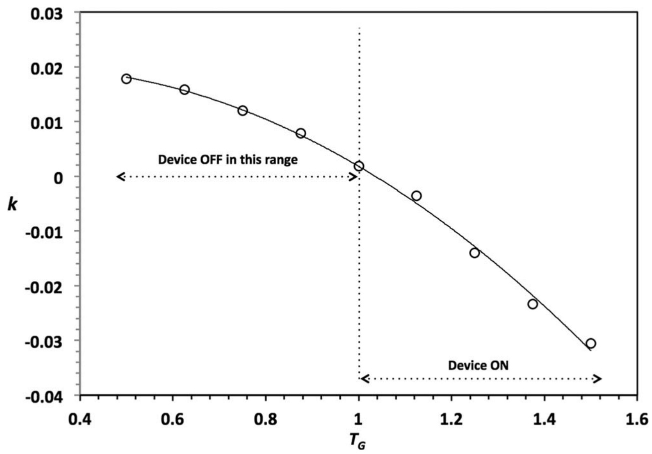

FIG. 3. The variation of the inverse resistance of the device, or its thermal conductivity, with changes in T_G. In the OFF state, the thermal conductivity of the device is positive whereas it is negative when the device is ON. Each dimensionless unit of temperature corresponds to 806 K while each corresponding unit of k is 5.29×10^{-9} W/K.

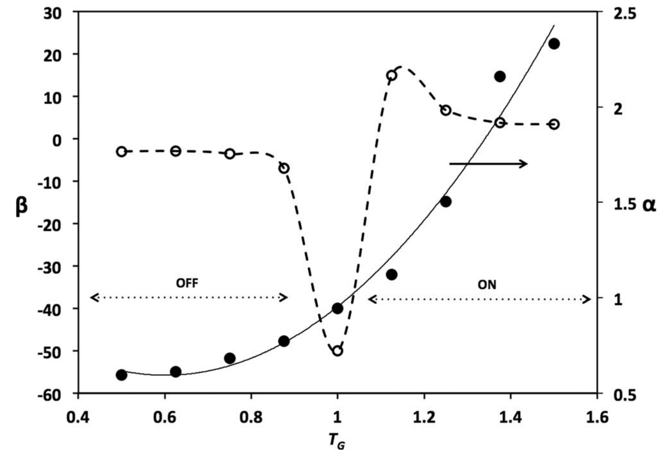

FIG. 4. The transport factor $\alpha = |Q_C/Q_H|$ and flux gain $\beta = -Q_C/Q_G$ with respect to varying T_G. The device is ON when $\alpha > 1$, i.e., more heat is rejected at the collector than is supplied to the emitter. It is OFF when $\alpha < 1$. The values of $|\beta|$ are roughly identical in both states although β is negative when the device is OFF and positive while it is ON. Each dimensionless unit of T corresponds to 806 K while β is dimensionless.

The thermal conductivity of the device is the inverse resistance $k = (1/R) = (Q_H + Q_C)/(T_H - T_C)$ based on the net current. Each dimensionless unit of k corresponds to 5.29×10^{-9} W/K. The variation of $k(T_G)$ is presented in Fig. 3. When $T_G = 1$, $k \approx 0$. In the OFF state, the thermal conductivity of the device, or its inverse resistance, is positive since the net heat current Q through the hot and cold terminals is also positive. Here, due to extraction through the gate, the hot terminal provides more heat current than is removed through the cold terminal. On the other hand, in the ON state $Q < 0$ so that k is also negative. This negative conductivity implies that more heat is extracted through the cold terminal than is provided at the hot terminal due to the intervention of the base terminal. The thermal conductivity variation is thus not an intrinsic material property. It results from the configuration of the device that exploits the nonlinear influence of the gate temperature on the heat extracted through the cold terminal. In practice, the device resistance can be varied by changing the wettability of the solid-fluid interface, e.g., by using UV light, or electrical or magnetic fields.[19] Negative thermal conductivities have been previously observed in systems with shape graded materials with thermal cloaks with various geometrical shapes[20] as well as chains of rotors where one rotor is attached to a thermostat and another to an external force.[21]

The nonlinear change in Q_C makes it possible to alter α and β by varying T_G, as shown in Fig. 4. If the direction of the current is identical through the base and collector terminals then β is negative, else it is positive. This device is similar to a three terminal electronic transistor where the base current is varied to change α and β. When the device is ON, $\alpha > 1$ since more heat is rejected at the collector than is supplied to the emitter. The transport factor is less than unity when the device is OFF. The absolute value of β is roughly the same in both states although it is negative when the device is OFF and positive while it is ON.

In summary, a relatively simple arrangement with three controlled temperature regions for a design involving a solid wall surrounding a sealed fluid leads to an effective thermal transistor. When $Q_C < Q_G$ and $Q_G < 0$, this device is OFF whereas it is ON when $Q_C < 0$ and $Q_G > 0$. The resistances in such a system could be readily varied by altering the solid-fluid wettability by making the walls more hydrophilic or hydrophobic.[7–10] A device based on thermal logic could lead to novel applications that consume significantly less energy by using waste heat to control the gate of the thermal transistor.

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