

Thermal rectification mechanisms including noncontinuum effects

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Abstract

Thermal rectification is a physical phenomenon where the resistance to heat flow is dependent on the sign of the temperature difference across a solid. This effect could be a useful phenomena to many industries if it could be controlled and optimized. However, experimental evidence shows that thermal rectification is dependent on a large number of competing factors. In addition, theoretical models that allow thermal rectification do not match measurements well largely because of the complexity of the effect and the immaturity of the models. Nevertheless, several mechanisms (geometric, electronic, electron-phonon scattering and anharmonic lattice vibrations) have been identified as possible means to control interface conductance at interfaces. Currently no evidence exists that suggests that the difference in conductance can reach one order of magnitude, which is an arbitrary limit required to deem the effect useful for engineered systems.

Mechanisms

Electron/phonon coupling New hypothesis (see below) valid for metal/insulator interfaces.

Geometric Rectification is achieved by changes in geometrical contact area often introduced by thermal expansion. Mechanism applies to

- macrocontact—surface mating, and
- microcontact—surface roughness.

Electronic Work function differences at interfaces can cause preferential flow of electrons leading to a self-biasing. If the electrons carry thermal energy, then rectification can be present.

- Can also be a function of oxidation at an interface where thermal transport is governed by tunneling electrons
- Model only valid for metals

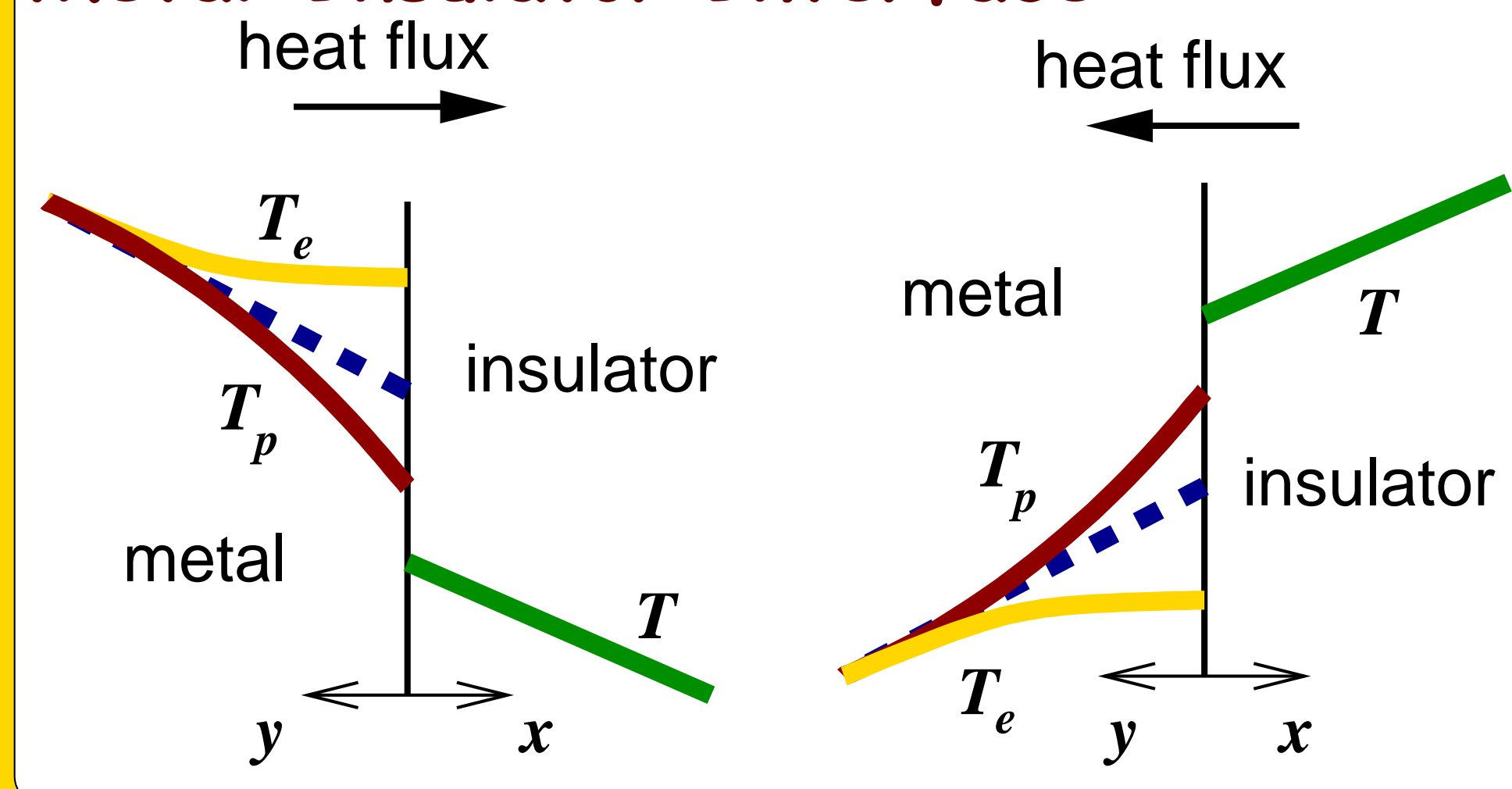
Phonon transmission Some non-symmetric feature of the interface prefers phonon transport in a given direction. Lattice dynamics and anharmonicity is required to achieve an effect. Can be geometry or material related.

Measurement error Interface phenomena are dependent on many things such as load, material treatment, interface preparation, interface cycling, temperature, materials, etc. Therefore, thermal rectification is difficult to verify.

Previous Works

Year	Author	Mechanism	Primary Finding
1936	C. Starr	unknown	The direction of highest conductance is from copper to oxide. Results were summarized by Henisch, 1949
1951	F.H. Horn	nonexistence	Horn suggested that Starr's observation was the result of the Thomson effect in uninsulated thermocouples.
1955	M.E. Barzelay, K.N. Tong and G.F. Holloway	electronic/geometric	Tests of composite airplane wings lead to an observation. Conductance is higher from aluminum to steel. This reference is unavailable, so conclusions contained in this work are surmised based on others' summaries.
1957	R.G. Wheeler	geometric	Thermal warping responsible for different conductance measurements.
1961	G.F.C. Rogers	electronic	Cites the Barzelay, 1955 results
1961	A. Williams	geometric	In response to Rogers, 1961, Williams states that the effect is likely due to surface contamination.
1962	R.W. Powell, R.P. Type and B.W. Jolliffe	nonexistent	Comparator tests found no directional effect of the order reported by Rogers, 1961. The tests involved a variety of loads as well.
1962	J.S. Moon and R.N. Keeler	electronic	described the electronic process by which rectification might occur. Also claimed that not enough data existed to draw conclusions about the magnitude of the effect.
1966	A.M. Clausing	geometric	rectification is a result of the difference in the expansion coefficient of two materials. Conductance of Aluminum to steel is larger and a function of load.
1968	D.V. Lewis and H.C. Perkins	geometric	Results showed that the directional effect is strongly a function of surface roughness. Results support Barzelay's and Clausing's conclusions.
1970	T.R. Thomas and S.D. Probert	electronic	steel and aluminum
1970	P.W. O'Callaghan, S.D. Probert and A. Jones	geometric	surface roughness effects
1982	D.L. Padgett and L.S. Fletcher	unspecified	rectification noticed at higher loads
1984	R.R. Somers II, L.S. Fletcher and R.D. Flack	geometric	developed geometric model to predict magnitude of thermal rectification based on expansion coefficients
1991	P.F. Stevenson, G.P. Peterson and L.S. Fletcher	geometric/electronic	Provides experimental evidence of both geometric and electronic contribution to rectification effects
1997	S.K. Parihar and N.T. Wright	unspecified	considered elastomer and metallic interfaces
2001	X. Sun, S. Kotake, Y. Suzuki and M. Senoo	phonon transmission	change in conductance is related to the temperature dependence of phonon transmission
2001	S.L. Lee and C.R. Ou	geometric	Numerical treatment of thermal contact conductance with thermal rectification
2002	M. Terraneo, M. Peynard and G. Casati	phonon transmission	Molecular dynamics study using highly nonlinear lattices show evidence of thermal rectification
2004	B. Li, L. Wang and G. Casati	phonon transmission	phonon mismatch at boundary leads to directionally dependent transmission
2005	D. Segal and A. Nitzan	phonon transmission	anharmonic atomic potentials lead to rectification
2005	C. Vanden Broek, P. Meurs and R. Kawai	nonequilibrium	Uses the concept of Brownian motors to explain thermal rectification
2005	D.G. Walker	nonequilibrium	energy gain/loss dependent scattering processes at and across interfaces responsible for rectification

Metal-Insulator Interface



Selected Results

$$\text{effectiveness} = \frac{(h_{\text{large}} - h_{\text{small}})}{h_{\text{small}}}$$

system	effect
Cu→Cu ₂ O, Starr, 1936	1.1
Al→SS, Rogers, 1961	0.2
Al→SS, Powell, 1962	0
SS→Al, Clausing, 1966	0.5
Al→SS, Lewis, 1968	1.4
smooth→rough, O'Callaghan, 1970	0.3
rough→smooth, Stevenson, 1991	0.52
metal→insulator, Walker, 2005	0.3

- The electron/phonon mechanism is based on several not well understood parameters, so magnitude of the effect is approximate.
- Because of dependence on many variables such as temperature and load, exact magnitude of rectification behavior is difficult to evaluate (and model).
- Large amounts of thermal rectification are difficult to achieve because of the incoherence (randomness) of thermal transport.

Electron/Phonon Coupling

Conductance (using Fermi's golden rule)

$$h = \frac{h_{ep}h_p}{h_{ep} + h_p} \quad h_{ep} \sim \left[\left(N_0 + \frac{1}{2} \mp \frac{1}{2} \right) g_c(E_e \pm E_p) \right]^{1/2}$$

- Directional effect from quantum mechanics:
 - Conductance is proportional to $N_0 + \frac{1}{2} \mp \frac{1}{2}$ where N_0 is the Bose-Einstein distribution and \mp depends on whether the process is energy loss or gain.
 - Heat flow from metal to insulator is an energy loss process and heat flow from insulator to metal is an energy gain process.
 - Effect is larger at low temperatures where N_0 is small.
- Directional effect from confinement:
 - A confined density of states ($g_c(E_e \pm E_p)$) could result in dramatic differences for energy loss and gain processes.

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