# 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

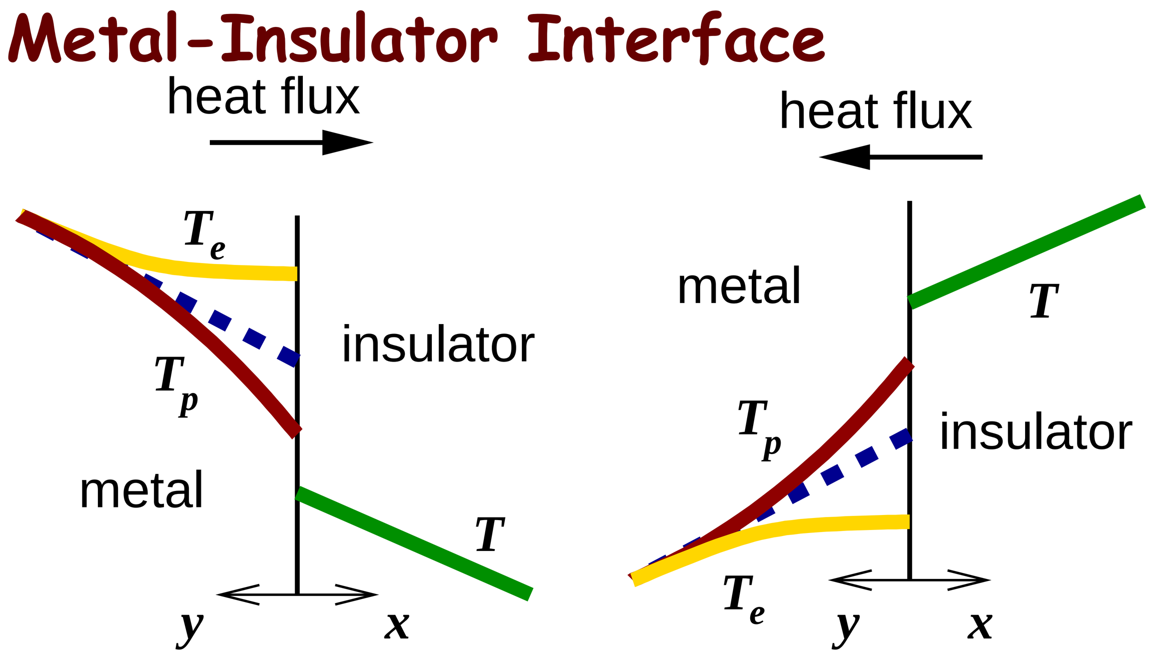
**Phonon transmission** Some non-symmetric feature of the interface prefers phonon transport in a given direction. Lattice dynamics and anhamonicity is required to achieve an effect. Can be geometry or material related.

**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 rectiifcation 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 od 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. Gasati | 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 recitification |
| 2005 | D.G. Walker | nonequilibrium | energy gain/loss dependent scattering processes at and across interfaces responsible for rectification |

## Metal-Insulator Interface




## Selected Results

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

| system | effect |
|---|---|
| Cu→$Cu_2O$, 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)

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

- Directional effect from quantum mechanics:
  - Conductance is proportional to $N_o + \frac{1}{2} \mp \frac{1}{2}$ where $N_o$ is the Bose-Einstein distribution and $\mp$ depends on whether the 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 $N_o$ 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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