Understanding Phonon Transmission in SrTiO3/PbTiO3 Superlattices Using Atomistic Green's Function

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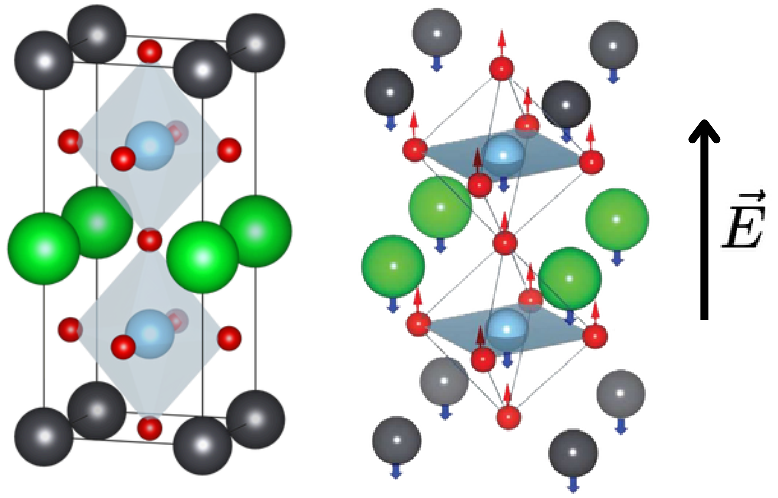
Introduction

Superlattice: Periodically layered structure of two or more materials



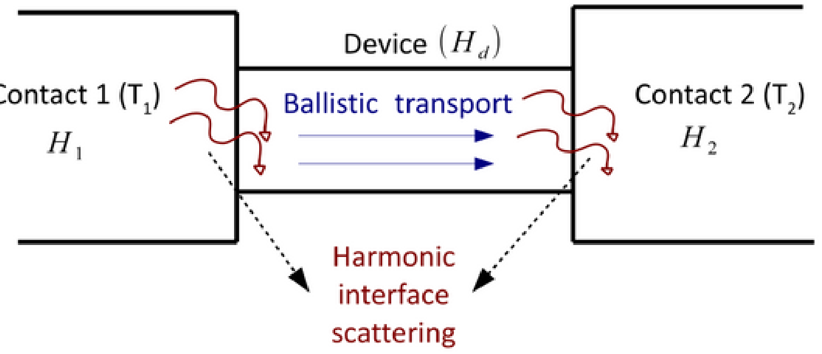
- Superlattices offer *tunable* thermal conductivity via layer thickness [1]
- Ferroelectrics offer a *controllable continuous range* of thermal conductivity using an external electric field [2]
- Domain walls can be *written* and *erased,* providing a dynamically modulating heat flux [3]

Used to *create*

- Efficient thermal management in microelectronics
- Energy harvesting devices
- Phononic computation and data storage technology

Methods

- Understanding phonon transmission across material interfaces allows us to understand heat conductivity in superlattices
- The atomistic Green's function (AGF) method calculates transmission probability $\mathcal{T}(\omega)$



Schematic of a typical phonon transport problem considered by AGF formulation. H represents the harmonic matrices of left isolated contact, device, and right isolated contact from left to right, respectively. [5]

Implemented theory using Python:

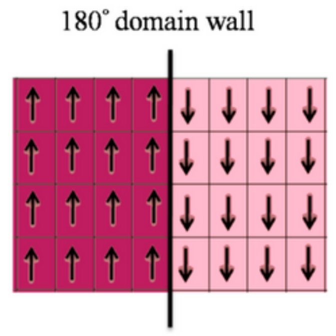
1.) Interatomic force constants calculated using Abinit and LAAMPS and extracted using Abipy.

2.) Construct harmonic matrices needed in AGF code.

$$J = \frac{1}{2\pi}\int_0^\infty \hbar\omega\mathcal{T}(\omega)[n_B(\omega,T_L) - n_B(\omega,T_R)]d\omega$$

Landauer expression relates heat current to transmission probability

3.) Subset of total Green's function needed for transmission probability calculated using Sancho-Rubio decimation scheme.



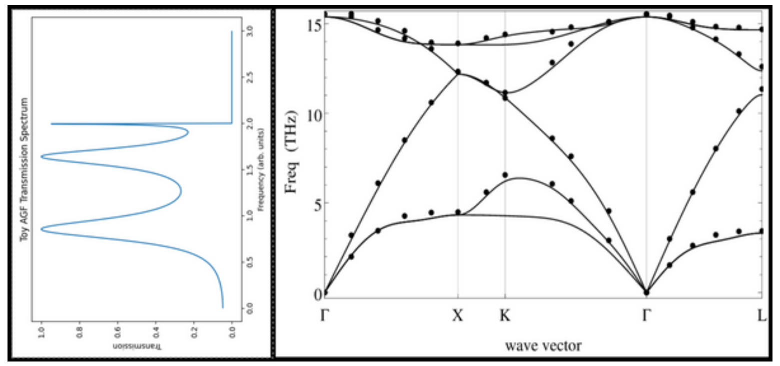
Example of domain wall (boundary between two regions with different electric polarizations) [4]

Experimental Setup:

- Use density functional perturbation theory as ground truth to simulate 1x1 interface and crude DWs
- Use LAAMPS (molecular dynamics) to simulate a more realistic response to the external electric field with machine learning potentials (MLIPS)
- Observe which phonon modes are filtered by the external electric field

Example

Transmission probability will give us an idea as to which modes contribute most to the head conductivity of the superlattice.



Future Work

In the future, I hope to

- Complete series of calculations
- Implement anharmonic extension of the atomistic Green's function method

References

[1] S. Chakraborty, C. A. Kleint, A. Heinrich, C. M. Schneider, J. Schumann, M. Falke, and S. Teichert, enThermal conductivity in strain symmetrized Si/Ge superlattices on Si(111), Applied Physics Letters **83**, 4184 (2003).

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[3] J. A. Seijas-Bellido, C. Escorihuela-Sayalero, M. Royo, M. P. Ljungberg, J. C. Wojdel, J. Íñiguez, and R. Rurali, enA phononic switch based on ferroelectric domain walls, Physical Review B **96**, 140101 (2017).

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[5] S. Sadasivam, Y. Che, Z. Huang, L. Chen, S. Kumar, and T.S. Fisher, enTHE ATOMISTIC GREEN'S FUNCTION METHOD FOR INTERFACIAL PHONON TRANSPORT, Annual Review of Heat Transfer **17**, 89 (2014).