Heat transfer across TiSi2(C54)/Si interface

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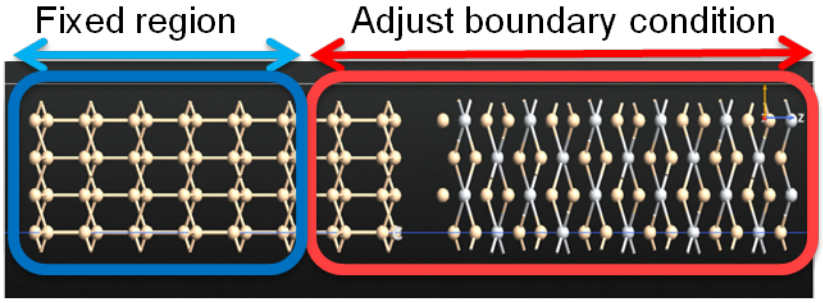
Objectives:

- Study the crystal structure relaxation of $TiSi_2$(C54)/Si interface.
- Calculate the thermal transport across interface.

Challenges:

- NEMO5 cannot generate some exotic crystal structures. ATK can.
- Interface effects are not accounted for strain, lattice mismatch and relaxation.

Method:



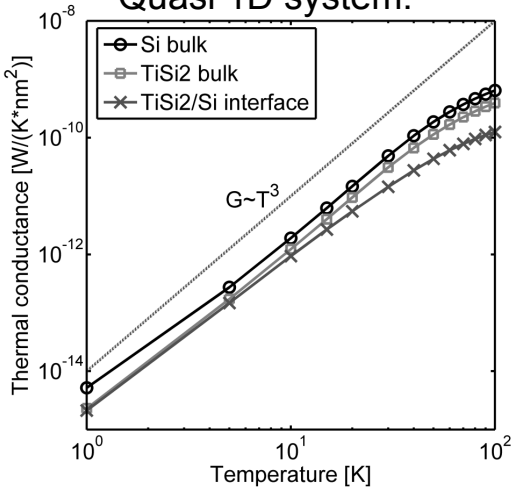
Relaxation happens around the TiSi2 (C54)/Si interface

1. New lattice structure is read into NEMO5.
2. Strain solver constructs the dynamical matrix.
3. RGF and NEGF are both available to do the transport calculation.

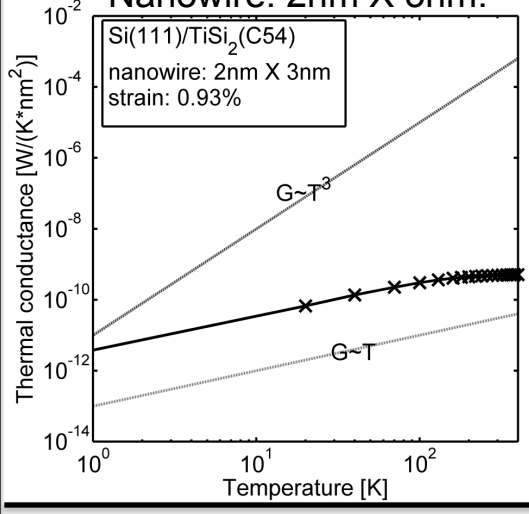
Results

- G has the T^3 dependence in low temperature.
- This is consistent with conventional theory and experiment result.

Quasi 1D system:



Nanowire: 2nm X 3nm.



Thermal conductance is temperature dependent due to the surface confinement.

Conclusions:

- An atomistic method with DFT+NEGF is first applied to simulate the heat transport across M/S interface.
- Thermal conductance with different boundary condition has different temperature dependence.