

Overview of phonon transport in NEMO5 Kai Miao, Prasad Sarangapani, Tillmann Kubis

Objectives:

- Implement phonon Büttiker probe in NEMO5
- Choose proper transport models
- Enable phonon transport with different methods

Challenges:

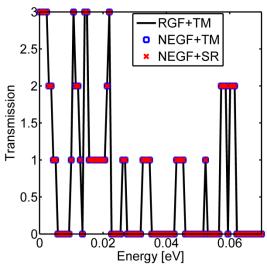
- Should understand all transport models
- Couple the strain solver with propagation class

Overview of phonon transport inNEMO5:

For phonon Büttiker probe simulation, Sancho Rubio +NEGF and General Lead+NEGF are 2 possible choices for:

- Transfer matrix cannot give flat particle density with scattering in both leads and device.
- Buettiker probe model needs the whole Hamiltonian matrix information in the device.

Result:



TM: Transfer matrix SR: Sancho Rubio Nanowire:6x1x1 (unit cells) Green's function

NEGF

RGF











Different transport methods are enabled in NEMO5.

Choose proper transport models for different aims.

