

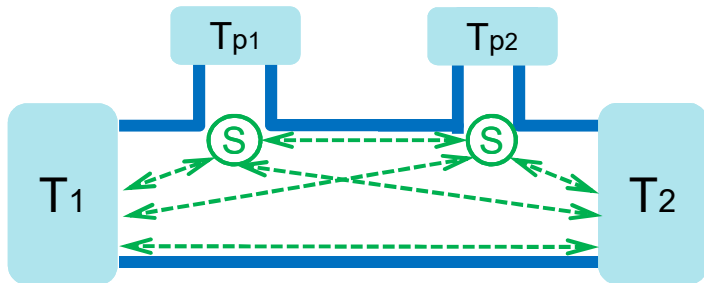
### ➤ Objective

- Study thermal transport across material interface via NEGF ✓
- Develop electron-phonon coupled transport model (ongoing)

### ➤ Challenges for NEGF

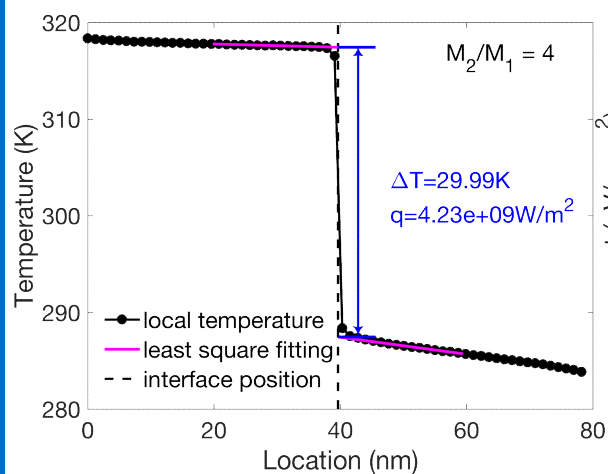
- Input force constant for phonon Dynamical matrix
- Efficient method for scattering
- Local temperature analysis

### ➤ Solution & Method

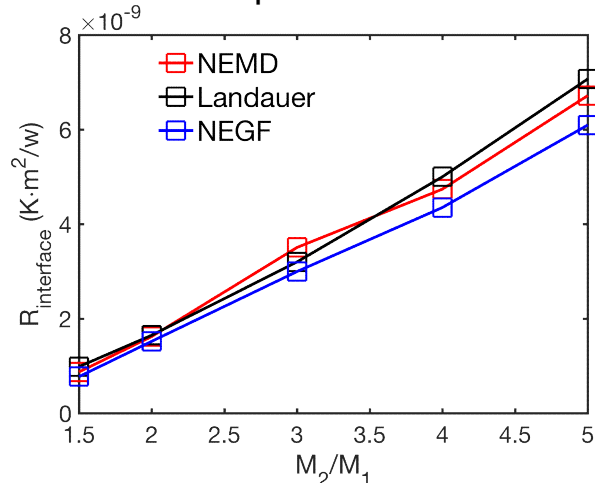


- Read in phonon potential from MD
- RGF compatible Büttiker probes for diffusive transport
- Phonon/Electron lifetimes from experiment data

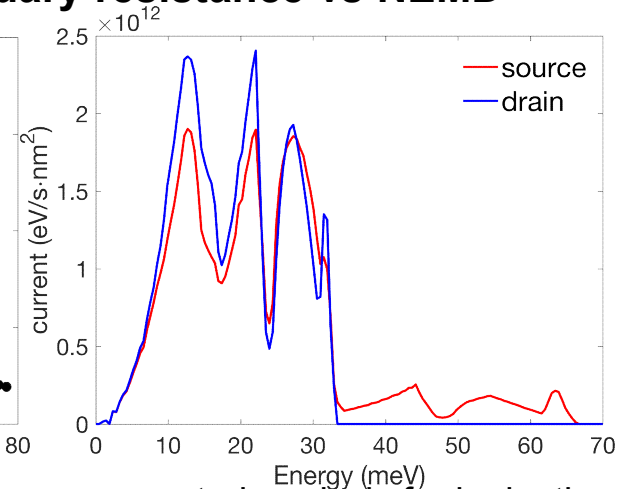
### ➤ Si/Heavy Si thermal boundary resistance vs NEMD



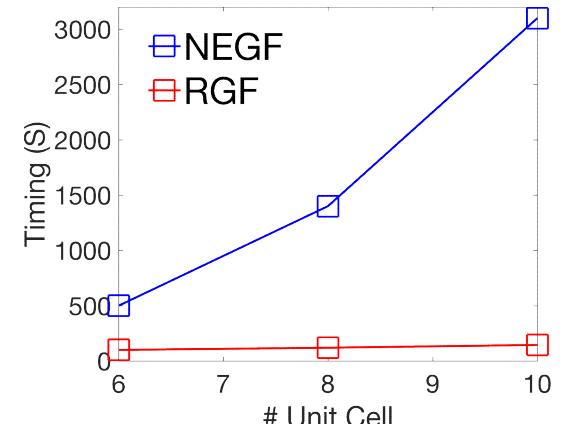
#### • Local temperature extraction



- Interface resistance agrees well with NEMD



#### • spectral analysis for inelastic scattering



- RGF greatly reduces computational expense

- Efficient Phonon diffusive transport model is developed
- Verified against NEMD method