Anharmonic Lattice Dynamics set of codes to model materials properties at high temperatures

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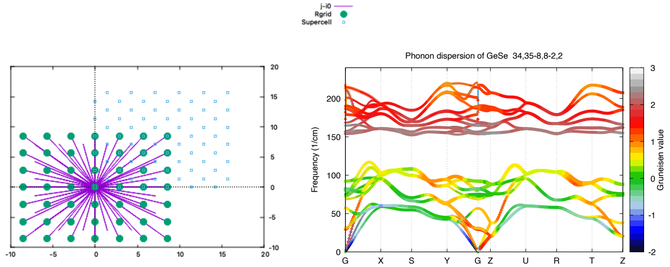
$$H^{model} = \Sigma_i \left(\frac{p_i^2}{2m_i} + \frac{1}{2}\Sigma_j\, \phi_{ij}\, u_i\, u_j + \frac{1}{3!}\Sigma_{jk}\psi_{ijk}\, u_i\, u_j\, u_k + \frac{1}{4!}\Sigma_{jkl}\, \chi_{ijkl}\, u_i\, u_j\, u_k\, u_l + \cdots\right) \qquad F_i^{model} = -\left(\Sigma_j\, \phi_{ij}\, u_j + \frac{1}{2!}\Sigma_{jk}\psi_{ijk}\, u_j\, u_k + \frac{1}{3!}\Sigma_{jkl}\, \chi_{ijkl}\, u_j\, u_k\, u_l + \cdots\right); \qquad J^\alpha = \frac{1}{2}\sum_{ij} R_{ij}^\alpha\, u_i^\beta v_j^\gamma (\phi_{ij}^{\beta\gamma} + \frac{2}{3}\psi_{ijk}^{\beta\gamma\delta} u_k^\delta + \cdots)$$

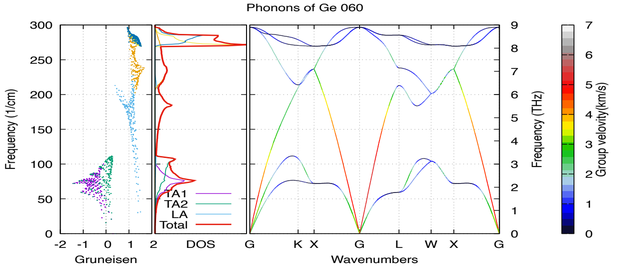
Force constants — Atomic displacements

FOCEX

Force Constant Extraction from a set of DFT calculations in a supercell

- Up to rank 8
- Can select range of each rank
- Can impose translational rotational and Huan invariance conditions
- Inputs can be from supercells of different shape and size.
- Also outputs phonons, DOS, elastic constants and Gruneisen

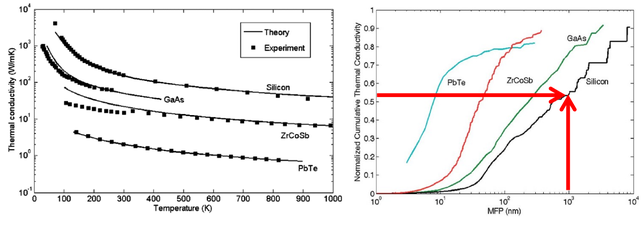




THERMACOND

Solves Boltzmann transport equation within and beyond relaxation time approximation

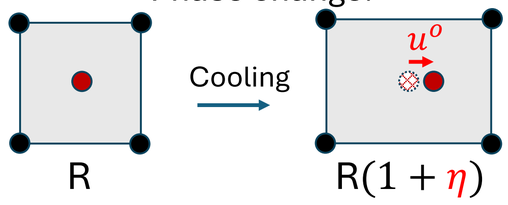
- Includes defect scattering (Tamura's formula)
- Uses full crystal symmetry, requiring only modes within the irreducible Brillouin zone.
- Efficient solution through CG minimization of $\frac{1}{2}Cf^2 + Df$ where C =Collision matrix ; f =phonon distribution function

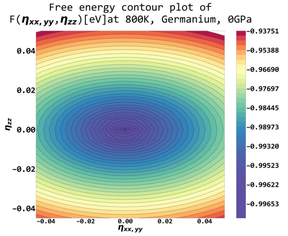


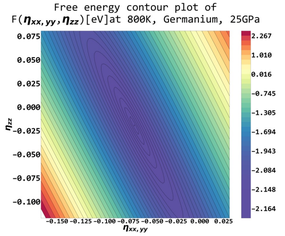
SCOP8

- Finds the state of thermal equilibrium at any given temperature using the Self-Consistent Phonon theory by minimizing a variational free energy $F(K, \eta, u^0)$
- $K(T)$ = effective harmonic force constant
- $\eta(T)$ = strain
- $u^0(T)$ = atomic relaxation
- Also outputs temperature-dependent phonon dispersion, Free energy, elastic constants, thermal expansion

Phase change:







ANFOMOD

Anharmonic FOrce field MOlecular Dynamics

Uses the anharmonic force field generated by FOCEX to do MD simulations and calculate the heat current.

Acknowledgement

For financial support through the CSSI program award #2103989

References

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https://aladyn.readthedocs.io/en/latest/run.html
https://github.com/KeivanS/Anharmonic-lattice-dynamics