PROJECT 1 : Study of lattice vibrations and thermal conductivity in disordered alloys

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1. The physics that we want to explore.

A first-principles theoretical study of lattice vibrational properties like, phonon dispersion, phonon density of states and thermal conductivity for disordered systems are always a difficult task. The difficulty is two-fold :

(i) The input dynamical matrices are always calculated either in the pure constituents or in the ordered alloy. Whereas we need to calculate it in a random background.

(ii) In dealing with configuration avergaing, the basic problem lies in the presence of diagonal and off-diagonal disorder of the dynamical matrix of the system. The standard mean-field approaches cannot deal with off-diagonal and related diagonal + off diagonal disorders.

2. What needs to be done :

(i) We shall simulate the disordered lattice by Zunger's SQS and calculate the dynamical matrices in this disordered environment. We will be using computer code "Quantum Espresso (A PWSCF based programme)" and "SQS (along with VASP)" to extract the force constant between the atoms in the SQS structure. It has been claimed that the SQS based generated force constant incorporate the disordered effect within it, so it would be a good starting point to the study of vibrational properties. Zunger *et.al.* first introduced a model to deal with disorder through SQS method. This basically design an N-atom per cell periodic structure so that their

distinct correlation functions $\Pi_{k,m}$ best match the ensemble-averaged correlation-functions $< \Pi_{k,m} >$ of the random alloy. After this an averaging procedure is done under the specified symmetry upon the force constant tensor matrices and finally this will be the input parameters for our ASR based method to study lattice vibrational properties.

(ii) The disorder configuration averaging we shall do using the ASR technique complemented by the ASR based ICPA. We shall get DOS, Spectral function, Life-times from this.

(iii) The thermal conductivity will be calculated using the Kubo formula based technique in augmented space.

All the codes and knowhow of this part has already been developed. It requires consolidation and application.

3. Going beyond one atom per unit cell.

Till now existing k-space AS-recursion dealt with only single atom per unit cell systems. Due to this we are constrained to simple stochiometric binary alloys. In this project we will introduce the many atom based k-space recursion so that we can deal with complex structures and describe non-stiochiometric alloys and partially disordered alloys (in which two penetrating sublattices have different disorders).

Work distribution

- Dynamical matrices through SQS - BS, SG
- DOS,SF using ASR - RKC, AM
- DOS,SF using ICPA - SG
- Thermal conductivity using AS - RKC, AA
- Multi-atom per unit cell - RKC, AA, AM