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Investigation of properties of alloys through multiscale computational modeling

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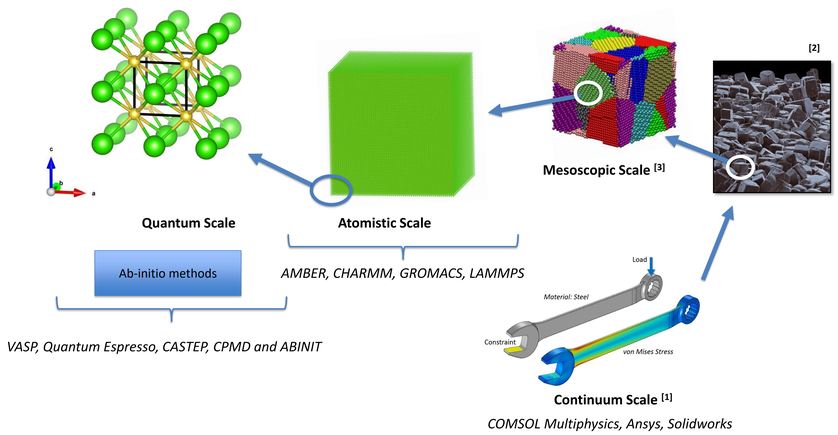
Abstract

Mechanical, electrical and thermal performance of the joints made between circuit components is heavily dependent on the soldering process and the soldering alloy. As Pb-based solders are being phased out from commercial use, research is being carried out to develop newer alloys to match the performance characteristics of Pb-based solders. Computational modeling has been widely used to investigate the performance of new alloy combinations, leading to the requirements for the development of multiscale modeling of an intermetallic joint. To determine the feasibility of such an efficient scaling process, we simulate mechanical and thermal characteristics across *ab initio* and classical molecular dynamic implementations. We employ *ab initio* modeling using density functional theory on a supercell and compare the results for the same structure using classical molecular dynamics. The outcome from the comparison of the results from the two methods is expected to enable us to investigate the role of multi-scale modeling in predicting the properties of alloys at improved rates while maintaining the accuracy of results.

Soldering

Soldering is the process of joining of two or more metals using solder as a filler material, having a long history running back a few millennia. Properties considered in designing a good soldering material include appropriate melting point, low thermal expansion, ductility, strength, resistivity, low susceptibility to corrosion, fatigue failure etc. It has had a profound impact on modern electronic circuitry from 1920s using Pb based solder. The most common mixture is a 60/40 (Sn/Pb) blend with a eutectic around 182°C. As Pb based solder is being phased out from use, Pb free solder materials need to be developed with similar properties. A common alternative is SAC (Sn-Ag-Cu) alloy with varying proportions such as SAC305/387/405. However these tend to have higher T_m compared to Pb based solder. Researches are also being done to develop Sn-Bi based solder alloys.

Scales of Modeling



Ab-initio, Semi-empirical, DFT Methods vs CMD

Ab-initio

- Latin for ``from the beginning''
- Computations that are derived directly from theoretical principles with no inclusion of experimental data
- Adequate only for small systems and are based entirely on theory from first principles including Schrodinger equation.
- Very high accuracy for minimal structures
- Very high computational cost, ~ few atoms

Semi-Empirical

- Approximations/omissions of some factors to ease computational effort such as core electron omissions, minimal basis sets, two electron integral omissions.
- Parameterization to estimate omitted values through ab-initio methods/experimental values.
- Comparatively faster
- Results rely on parameterization values and molecules used to parameterize.
- ~ 100 Atoms

Density Functional Theory

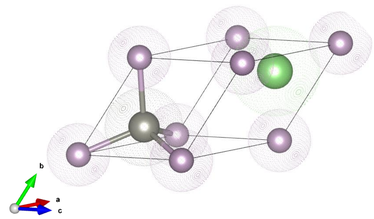
- Electronic structure is analyzed using a potential acting on the electrons, constructed as the sum of external potentials V_{ext}, which is determined solely by the structure and the elemental composition of the system, and V_{eff}, representing interelectronic interactions.
- Supercell of a material with n electrons is treated as a set of n Schrödinger-like equations, also known as Kohn–Sham equations.[4]
- Very efficient in calculations with accurate results.
- Difficult to accurately model intermolecular interactions, charge transfer excitations etc.

Classical Molecular Dynamics

- Solution of the classical equations of motion for atoms and molecules to obtain the evolution of a system with time.
- Requires pre-established potential energy parameters which are derived/fitted for specific conditions. Inter-usability of force-fields for mixed environments is dependent on many conditions.
- Do not account for electronic properties.
- Computationally cheap compared to first principles methods.
- Accuracy of results depend on the quality/suitability of parametrization, computational process (coding) accuracy and "bulk" of the simulation.

Computational Work

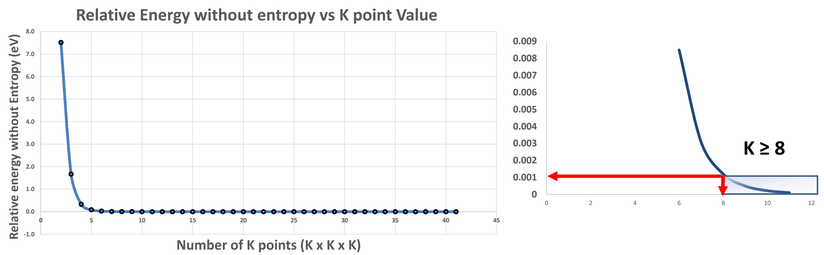
The positional data for **LiZnP** was obtained [2] and was used for the study of selection of optimal K points to sample the Brillouin zone, and the optimal energy cutoff (ENCUT) values using VASP®. The time spent per each calculation was also plotted as a measure of the computational cost. The node used for calculation was kept constant for each analysis.



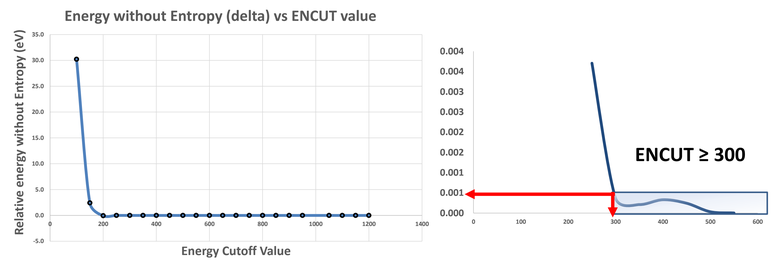
Results

- Optimal number of K points to be used to sample the Brillouin zone – 8x8x8
- Converged ENCUT parameter for the system is 300 eV
- Effectivity of the parallelization of the program(scaling) for the PLZ system is best at 8 cores per computation task.

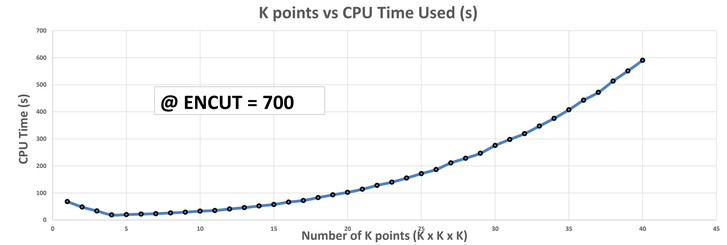
Calculating the optimal K points



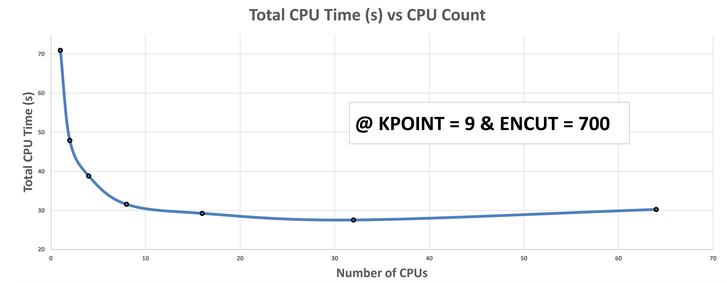
Calculating the optimal Energy Cutoff Values



Variation of Processing time with No. of K Points



Variation of Processing time with No. of Computing Cores



Future Plans

The variation and optimization of the above results with respects to parallel computing architecture (effects of oversubscribing, hyperthreading etc.), and types of system remains to be investigated. Immediate projects in the pipeline include calculation of the elastic properties of solder alloys and benchmarking the individual techniques with the size of the system. This will then be extended to study Sn-Bi solder alloys and their elastic properties with a system size of ~100 atoms based on DFT. In due course the researchers intend to develop/link the results from DFT calculations and atomistic simulations for a comprehensive study on multi-scale computational methods to study the properties of alloys.

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