

Development of ab-initio multibody energy expansions for the design of metallic materials with extremal properties

EXECUTIVE SUMMARY

Concepts of materials-by-design developed recently have allowed exploration of the range of properties attainable by tailoring the microstructural features of the material. In particular, by changing the volume fractions of various crystal orientations, or by tailoring the placement of these crystal orientations in the microstructure, it is possible to achieve a range of properties. However, this range is restricted by the anisotropy of the single crystal. For example, in FCC Copper, the elastic modulus of any given polycrystal is bounded between 66 GPa to 191 GPa, which correspond to the limits of single crystal Young's modulus. However, alloying copper with a relatively cheaper material like zinc can provide up to 35% increase in the range of obtainable properties. The proposal aims to explore such variations in compositional degrees of freedom for designing materials in conjunction with the microstructure design approach from our earlier ARO-supported work.

Experimental as well as complete ab-initio methods for identifying best alloy phases are hindered by the combinatorial complexity of compositional space. In this proposal, we develop a generalized potential expansion constructed with ab-initio data that provides a scalable method for computing stable structures and their thermo-mechanical properties. Here, the formation energy of a multiple atom system is efficiently found by representing it using energies of small isolated clusters. The problem of constructing such potentials is addressed through development of adaptive sparse-grid interpolation. This technique, unlike existing techniques, enables identification of new stable phases (e.g. Laves phases) with exceptional anisotropies that may not fall within the parent FCC, HCP or BCC lattices. Compositions with desired properties are obtained by constructing iso-contours of properties in compositional space using active sampling techniques.

The properties of the designed material will then be utilized in our existing microstructure-design framework to construct property closures using homogenization and optimization techniques. The technique allows us to identify the combination of phases that is most likely to result in desired set of properties along a given loading direction. These following key points are addressed:

- ✚ Adaptive sparse-grid technique for efficient and accurate interpolation of cluster energies.
- ✚ Computation of properties of stable phases using multi-body expansion.
- ✚ Multi-property closures for identification of the range of obtainable properties from the polycrystal made from the new material using microstructure-sensitive-design methodologies.
- ✚ Development of a database of promising structures and associated property maps that experimentalists can take advantage of.

Impact to the U.S. Army: The materials-design technique developed will be able to support the increasing need for exceptional materials for structural use pertinent to the U.S. Army. Key applications include the development of high performance protective structures with optimized stiffness, low thermal resistance and high phase stability.

Broad technical impact: Owing to the generalized nature of the proposed mathematical developments, this framework can be extended to design materials with tailored electrical, optical and magnetic properties for specialized applications. By disseminating algorithms and databases, we will enable broad research communities to apply such techniques for materials design.

Educational impact: A newly introduced graduate course offered by the PI on atomistic modeling of materials that serves the engineering, physics and chemistry communities at Cornell will be enhanced with the proposed activities by allowing many graduate students to participate with hands-on computational experience in electronic structure calculations and their relation to properties and processes of engineering materials.