Project Report FY 2016

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II. Summary of research projects:

Following are the summaries of the research projects that we are currently working on:

- *Design of high strength advanced steels*: aims to predict optimum temperatures for two-step heat treatment to maximize the retained austenite in TRIP steel by employing a three pronged approach: (1) heat treatment design using genetic algorithm coupled with computational thermodynamics, (2) modeling of plastic flow behavior and (3) Bayesian parameter and uncertainty calibrations. The goal is to minimize the cost of the research and development of the materials, which would be otherwise high if it was entirely conducted by means of experiments.

- *High temperature shape memory alloys (SMAs)*: the goal is to understand the fundamental behaviors of the materials such as magnetic and structural transformations, magneto-caloric and elasto-caloric effects, and formation of spins and strain glass in SMAs using first-principles calculations and Monte Carlo. Such understanding would tentatively help to better control the phase transformations and microstructure formations of the materials during experimental processing for enhanced properties and performances.

- *Metallic fuels*: investigations of the effects of thermodynamics and kinetics of actinide and fission products on the phase stability and microstructural evolutions of the nuclear fuels. The particular system of interest is U-Nb. This system exhibits a wide range of bcc phase region and a high melting point which promise stable chemical and mechanical operating conditions for nuclear reactor at elevated and high temperatures. However, under various low temperature heat treatment conditions, it undergoes various microstructural transformations which affect the properties of the fuel. The current research tries to understand one of the transformations, known as discontinuous precipitation which tends to reduce the fuel corrosion resistance and ductility. The approach is a multi-scale multi-physic coupling of quantum-based calculations, computational thermodynamics, and phase-field microstructural modeling.

- *Lead-free soldering*: aims to substitute lead soldering by Cu-Sn and Cu-Sn-Ag soldering. The later even though is environmental friendly exhibits microstructure evolutions which tend to affect the mechanical properties of the soldering. To understand the fundamental thermodynamics and kinetics governing these microstructural evolutions, the use phase-field modeling is proposed. This approach couples thermodynamics and kinetics in a self-consistent way and so far has demonstrated satisfactory result in comparison with experiments. Currently, it is extended to couple additional physics to better assess the system under various conditions including internal stress/strain field, electro-migrations, and void formation.

- *Materials Informatics and Design*: development of a materials database and curator to facilitate materials design. The database would contain basic properties of materials which can be assessed by quantum mechanical calculations. The focused materials at the current stage are SMAs and MAX phases, which promise many interesting and practical applications. It is hoped that the exploitation of these data via materials informatics would yield interesting physical, chemical, and mechanical relationships which are essential for the optimization of the materials' properties.

III. Publications (in FY 2016):

1. Anjana Talapatra, R. Arroyave. Investigation of the energetics of structural transformations in Co-based shape memory alloys. Journal of Alloys and Compounds 663(2015), 693–700.
2. Anjana Talapatra, R. Arroyave, P. Entel, I. Valencia-Jaime & A. H. Romero. Stability analysis of the martensitic phase transformation in Co2NiGa Heusler alloy. Phys. Rev. B 92(5 2015), 054107.
3. R. Arroyave, Anjana Talapatra, L. Johnson, N. Singh, J. Ma & I. Karaman. Computational Thermodynamics and Kinetics-based ICME Framework for High Temperature Shape Memory Alloys. Shape Memory and Superelasticity 1.(4) (2015), 429–449
4. Attari, V. & Arroyave, Phase Field Modeling of Joint Formation During Isothermal Solidification in 3DIC Micro Packaging. R. J. Phase Equilib. Diffus. (2016) 37: 469.
5. Li, S., Honarmandi, P., Arróyave, R., & Rivera-Diaz-del-Castillo, P. E. J. "Describing the deformation behaviour of TRIP and dual phase steels employing an irreversible thermodynamics formulation." Materials Science and Technology 31.13 (2015): 1658-1663.
6. Honarmandi, P., & Arroyave R. "Bayesian Calibration of a Physical Model for Plastic Flow Behavior of TRIP Steels." TMS 2016: 145 Annual Meeting & Exhibition: Supplemental Proceedings. John Wiley & Sons, Inc.
7. Thien C. Duong, Robert E. Hackenberg, Alex Landa, Pejman Honarmandi, Anjana Talapatra, Heather M. Volz, Anna Llobet, Alice I. Smith, Graham King, Saurabh Bajaj, Andrei Ruban, Levente Vitos, Patrice E.A. Turchi, Raymundo Arroyave, Revisiting Thermodynamics and Kinetic Di□usivities of Uranium Niobium with Bayesian Uncertainty Analysis, Calphad (under review) 2016.

IV. Potential applications:

- *Design of high strength advanced steels*: steels are so far one of the main factors empowering industrial and social developments. It is hoped that via this work we could improve the processing conditions under which steels with enhanced mechanical properties can be synthesized. Also, we hope to establish a computational-based routine to reduce the cost and time of materials research and development of steels.

- *High temperature shape memory alloys (SMAs)*: shape memory alloys promise innovative technologies such as new sensors, actuators, and electromagnetic devices; new energy conversion and harvesting methods, new concepts for solid-state thermal management and thermal expansion compensation; and new principles for storage devices. It is hoped that via a better understanding of fundamental behaviors of SMA, promised by our current researches, it could help to accelerate the research and development of these materials.

- *Metallic fuels*: metallic fuels are excellent candidates for the next-generation nuclear reactors (Gen-IV). They promise higher energy efficiency and at the same time are very friendly to the living environment (since the fuels can be burned all the way to minor actinides, which can further recycled for new fuel loops therefore promise minimal-to-none hazardous disposals as well as proliferation risk). The research and development of such fuels therefore could help to strengthen the national energy security as well as economy.

- *Lead-free soldering*: new lead-free soldering would minimize negative impacts of soldering on the environment. Via the inherent microstructural joints, formed by intermetallic compounds during soldering solidification, the properties and performances may also be enhanced.

- *Materials Informatics and Design*: a rich materials database would empower the research and development of materials by mean of materials informatics. It is one of the fundamental to effectively accelerate the discoveries of innovative materials, which, according to the US Materials Genomics, would potentially strengthen the competitiveness of the nation.