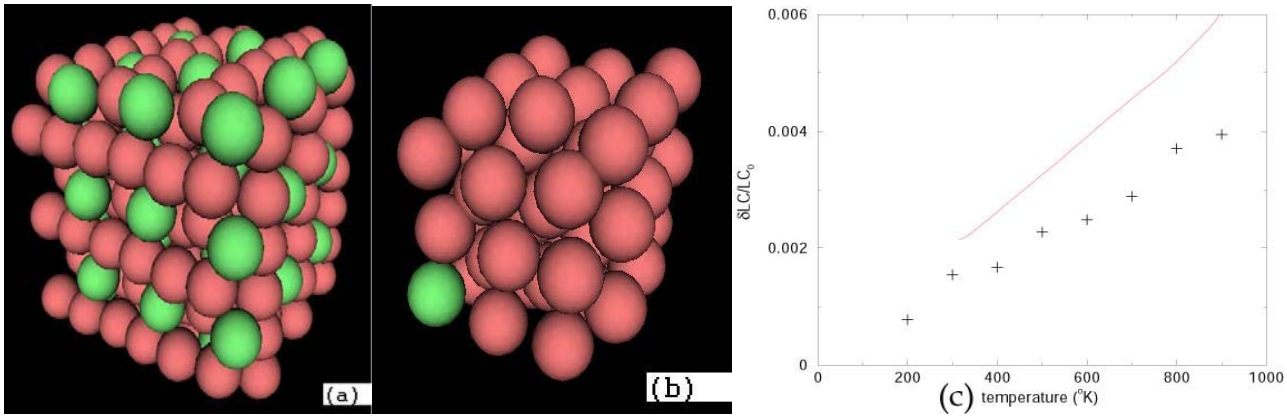

(a) Mo_3Si system (A15 structure, 216 atoms), snapshot taken after 50,000 Monte Carlo steps at 1200°K.
(b) Mo system (b.c.c. structure, 1 out of 54 atoms is replaced by Si), snapshot taken after 200,000 Monte Carlo steps at 400°K.
(c) CTE of system (b). The pluses are calculated by TB Monte Carlo, and the red curve is the experimental data.

Integrated Research For Predicting Higher Dimensional Phase Diagrams With Emphasis on Ternary Diagrams of Molybdenum, Silicon, and Boron

Associate Professor Bruce S. Kang, Department of Mechanical and Aerospace Engineering
Benedum Professor Bernald R. Cooper and N. Ma Department of Physics, West Virginia University.

The objective of this project is to develop and evaluate behavior of molybdenum silicide alloys for land-based power plant turbines able to withstand temperature exceeding 1000ºC. In addition to relevant experimental work, the major task is computational modeling studies of ternary system of Molybdenum, Silicon and Boron over a wide range of temperature.

Founded by the classic work of Slater and Koster half a century ago, the tight-binding (TB) methods have experienced a renewed popularity in recent literatures. The success of TB is not only due to its apparent advantage of theoretical simplicity and numerical efficiency, but also because it is a method that uses the direct real-space (as opposed to k-space) approach, and thus it has a wide range of applications in problems that lack perfect crystalline symmetries (e.g., defects, impurities, surfaces and interfaces). Compared to other empirical methods (such as classical potential or embedded atom method), TB is based on the quantum mechanical formulation and is thus believed to be more accurate to describe complicated materials such as transition metals. In this project, we developed a new TB scheme that is especially suitable for modeling of compound alloy materials. Using Mo_3Si as an example, we obtained the Slater-Koster TB parameters *directly* through results of full-potential linear muffin-tin orbital method by using a modified McMahan and Klepeis' approach. The transferability and accuracy of these parameters were tested against *ab initio* results. Furnished with a fitted repulsive energy that takes the form of embedded atom potential, the method was applied in Monte Carlo simulations to compute the coefficients of thermal expansions (CTE). The calculated results are in good agreement with our experimental results. **This is the first reported success of Monte Carlo or molecular dynamics simulation based on quantum mechanics energy method on inter-metallic binary alloys**.

Read more about this work.