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Accelerated material design

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New refractory alloys are critically required to increase lifetime and improve the efficiency of fossil and nuclear energy systems. The development of these materials remains slow because it is driven by a trial-and-error experimental approach and lacks a rational design approach. Atomistic multi-scale design has the potential to accelerate the alloy development through the predictive modeling of mechanical properties and corrosion resistance of new materials. The success of atomistic simulations depends critically on its ability to accurately account for chemical reactions, predict mechanical properties and handle large atomic systems within a reasonable time frame. Traditional Quantum Mechanics (QM) approaches are too computationally expensive and, therefore, can handle only very small atomic systems typically at the sub-nano level. This critical issue was successfully addressed in this work by developing, demonstrating, and validating a multi-scale framework with the following components: (i) first-principles Density Functional Theory (DFT) total energy analysis, (ii) Molecular Dynamics (MD) – Monte Carlo (MC) hybrid simulation technique, and (iii) ReaxFF reactive force field scheme that bridges the two. To demonstrate the feasibility of our first-principles-based approach, we have developed ReaxFF potentials for Al/Ni/Fe interactions. First-principles data from QM calculations such as energies and bulk structures were used for the evaluation of the ReaxFF parameters. QM calculations were performed by PAW method using VASP. The phase stability and the lattice parameters were calculated for the selected structures. We have concluded that the developed ReaxFF potentials for Fe-Ni-Al alloy systems are reliable to the scale of 3 kcal/mol•per atom for energy formation and correctly describe the thermodynamics of various bulk and surface structures. A direct comparison of ReaxFF-MD/MC simulation results with the measured surface segregation of Al for a FeAl (001) slab will be reported.

Biography

Alex V. Vasenkov is Senior Principal Scientist at CFD Research Corporation. He received his Ph. D. degree in thermophysics and molecular physics from the Russian Academy of Science in 1996. With 15 years of experience, he is an expert in material design, self-assembly processing of nanomaterials, and multi-scale modeling. His research was funded by federal agencies (NSF, DOE, and DoD) and industry (Samsung Advanced Institute of Technology, etc.). He is the co-author of a book chapter on multi-scale modeling of materials and over 30 publications in peer-reviewed journals.

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