Software Package Completed for Alloy Design at the Atomic Level

As a result of a multidisciplinary effort involving solid-state physics, quantum mechanics, and materials and surface science, the first version of a software package dedicated to the atomistic analysis of multicomponent systems was recently completed. Based on the BFS (Bozzolo, Ferrante, and Smith) method for the calculation of alloy and surface energetics, this package includes modules devoted to the analysis of many essential features that characterize any given alloy or surface system, including (1) surface structure analysis, (2) surface segregation, (3) surface alloying, (4) bulk crystalline material properties and atomic defect structures, and (5) thermal processes that allow us to perform phase diagram calculations. All the modules of this Alloy Design Workbench 1.0 (ADW 1.0) are designed to run in PC and workstation environments, and their operation and performance are substantially linked to the needs of the user and the specific application.

In response to the diverse needs of the scientific community, this tool, with the BFS method at its core, provides a simple and straightforward approach for gaining understanding of the properties of materials by increasing knowledge of the system behavior at the atomic level. In what constitutes a substantial improvement over alternative quantum approximate methods with comparable computational simplicity, the BFS method for alloys is free from most of the constraints on other techniques, such as limitations in the number and type of atomic species that can be accommodated or an inability to deal with arbitrary crystal structures. This results in a general, transferable, and accurate tool for examining the characteristics of multicomponent systems.

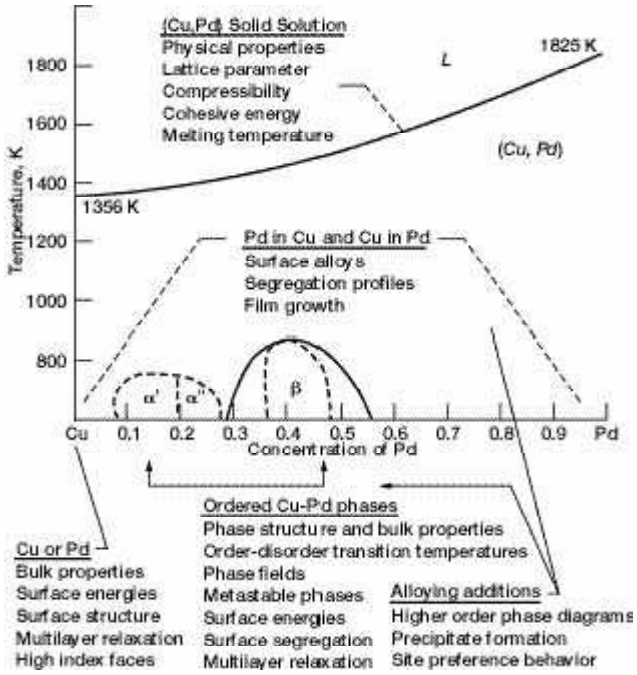
In the last few years, the BFS method for alloys, developed at the NASA Glenn Research Center, has been tested and applied to a large number of fundamental problems with consistent success (refs. 1 to 3). Because of the strong foundation of its general formulation, the simplicity of its implementation, and its computational economy, the method has proven to be a powerful and useful tool to aid in the process of alloy design and analysis. Although there are no limitations on the number of elements involved in the calculations, the crystal structure, or the input compositions, the current version of ADW is parameterized and can perform calculations with 15 elements in body-centered cubic form, 12 in face-centered cubic form, and 2 in the diamond structure. This data base is being updated constantly.

ADW 1.0 is available at Glenn for internal use by the Computational Materials Group. We envision that interaction with potential collaborators will help us to expand the scope and capability of this tool. Eventually, such collaborations and interactions with individuals and institutions will be instrumental in leading to a generally available software package.

The BFS method is extremely economical in the input needed, which is completely provided by first-principles calculations (linearized augmented plane wave method) without reference to any experimental data. Moreover, the small number of parameters

needed (three for each single element, two for each element pair), together with the universal nature of these parameters (i.e., applicable, without adjustment, to any problem dealing with these elements in a given symmetry, even in the presence of additional elements), make the BFS-based predictions surprisingly general given the limited input and the severe transferability constraints imposed on the parameters.

The package includes tools for developing large-scale atomistic simulations using Monte Carlo methods, as well as tools for performing analytical calculations based on user-defined catalogues of specific atomic configurations, which provide insight into the basic features of a given system on an atom-by-atom basis.



ADW 1.0 modules available for atomistic calculations of multicomponent metallic systems, illustrated by the applications related to the different regions of the Cu-Pd phase diagram (ref. 4).

The figure summarizes the type of information that has been determined using ADW 1.0 on an example binary system such as Cu-Pd (ref. 3).

1. Analyzing the bulk and surface properties of pure elements, including surface energies, surface structure, reconstruction, and multilayer relaxation

2. Forming surface alloys for any level of coverage, thin film structure and growth patterns, and interdiffusion into pure crystals

3. Identifying the segregating species and determining the driving mechanisms for segregation, surface segregation profiles, and their dependence on temperature, concentration and alloy crystal face, and alloy surface energies and structure

4. Determining bulk alloy crystal structure and properties including phase fields, order-disorder transitions, and critical temperatures

5. Determining the energetics of point and other atomic defects

6. Predicting and analyzing metastable structures

7. Determining physical properties such as lattice parameter, compressibility, and cohesive energy as a function of composition and temperature

8. Determining the role and behavior of ternary and higher order alloying additions, their site preference behavior, the formation of other phases, and the partitioning of the alloying additions to these phases

In summary, the first version of ADW, a software package dedicated to the atomistic analysis of multicomponent systems, was recently completed in response to the diverse needs of the scientific and engineering community.

References

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Additional references (http://www.grc.nasa.gov/WWW/SurfSci/bfs/bfs_index.html)

Ohio Aerospace Institute contact: Dr. Guillermo H. Bozzolo, 440-962-3103 or 216-433-5824, Guillermo.H.Bozzolo@grc.nasa.gov
Glenn contacts: Dr. Ronald D. Noebe, 216-433-2093, Ronald.D.Noebe@grc.nasa.gov; Dr. Phillip B. Abel, 216-433-6063, Phillip.B.Abel@grc.nasa.gov; and Dr. Brian S. Good, 216-433-6296, Brian.S.Good@grc.nasa.gov
Authors: Dr. Guillermo H. Bozzolo, Dr. Ronald D. Noebe, Dr. Phillip B. Abel, and Dr. Brian S. Good

Headquarters program office: OAT
Programs/Projects: HOTPC
Special Recognition: Reference 1 was named Glenn Research Center's Distinguished Paper of the Year for 1999.