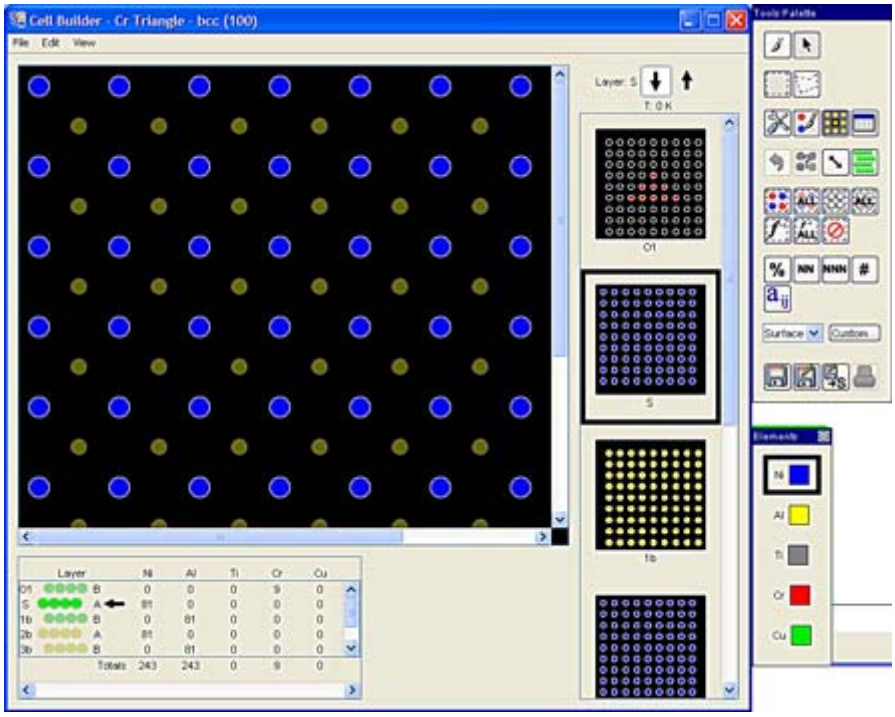
adwTools Developed--New Bulk Alloy and Surface Analysis Software for the Alloy Design Workbench

A suite of atomistic modeling software, called the Alloy Design Workbench, has been developed by the Computational Materials Group at the NASA Glenn Research Center and the Ohio Aerospace Institute (OAI). The main goal of this software is to guide and augment experimental materials research and development efforts by creating powerful, yet intuitive, software that combines a graphical user interface with an operating code suitable for real-time atomistic simulations of multicomponent alloy systems. Targeted for experimentalists, the interface is straightforward and requires minimum knowledge of the underlying theory, allowing researchers to focus on the scientific aspects of the work.

The centerpiece of the Alloy Design Workbench suite is the *adwTools* module, which concentrates on the atomistic analysis of surfaces and bulk alloys containing an arbitrary number of elements. An additional module, *adwParams*, handles ab initio input for the parameterization used in *adwTools*. Future modules planned for the suite include *adwSeg*, which will provide numerical predictions for segregation profiles to alloy surfaces and interfaces, and *adwReport*, which will serve as a window into the database, providing public access to the parameterization data and a repository where users can submit their own findings from the rest of the suite.

The entire suite is designed to run on desktop-scale computers. The *adwTools* module incorporates a custom OAI/Glenn-developed Fortran code based on the BFS (Bozzolo-Ferrante-Smith) method for alloys, ref. 1). The heart of the suite, this code is used to calculate the energetics of different compositions and configurations of atoms.



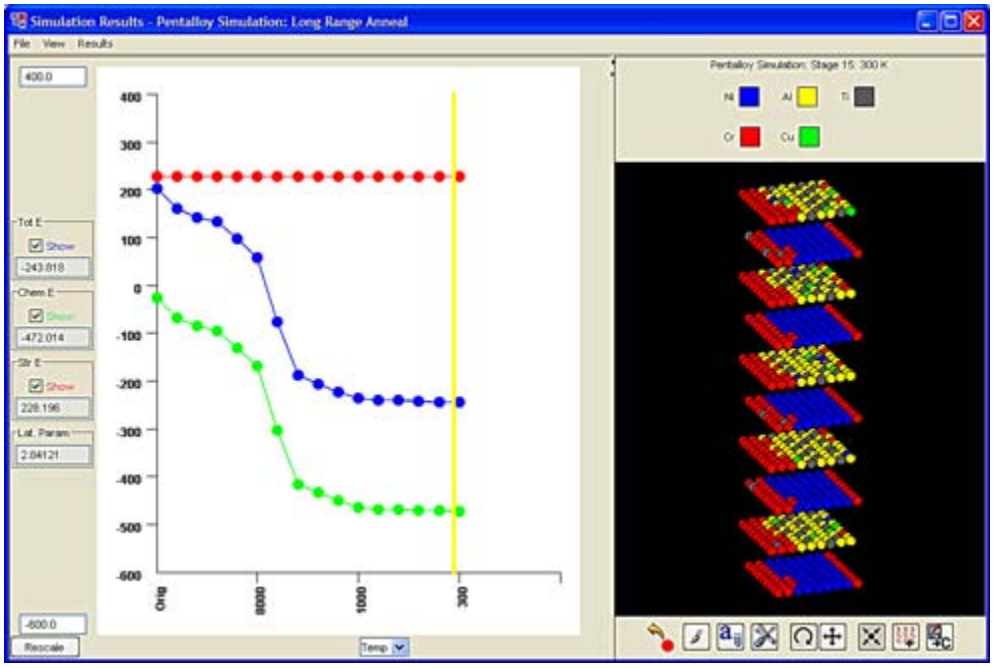
The starting point of adwTools is the cell builder, where arbitrary computational cells can be created using an extensive menu of options. These include several possible "Select" options for populating a lattice, as well as additional tools to make visualization easier.

Long description. Representative screen capture showing the cell builder has one layer of the cell enlarged for editing in the upper left two-thirds of the panel. Thumbnail images of the other layers are displayed in an adjacent, scrollable selection column. Editing tool buttons and an atomic element palette and legend form the right boundary. A scrollable table of statistics per layer is below the enlarged to-be-edited layer depiction.

The first step in using the *adwTools* module is to create a project, within which a user can define the structure and composition of computational cells, as illustrated in the preceding screen capture. Projects contain two types of analytical tools: catalogs and simulations. Both utilize the cell builder module, which provides tools for the creation of cells (e.g., multiple atom selection, layer selection, fill by species, random distributions, etc.). Layers can be added or removed, and antiphase boundaries can be created. Analysis tools allow for atom-by-atom understanding of the energetics underlying the modeled behavior.

Within a A HREF="http://www.icmsc.org/RT/catalog.html">catalog, a user can collect individually modified cells and compare their energies of formation. This analytical approach facilitates the comparison of different atomic configurations that can represent different compositions or atom locations. Energy calculations are done in real time (0.25 msec/atom in a standard Pentium III desktop personal computer). The results viewer displays all the cells in a catalog, along with an energy level spectrum that provides a ready reference for the difference in energy between different states (cells).

In addition to the analytical catalog approach to alloy bulk or surface energetics, adwTools provides several simulation tools. A simulation allows a user to create a cell and define a temperature cycle for a canonical ensemble exchange Monte Carlo algorithm leading to an equilibrium configuration, or relax the atomic coordinates via multiple relaxation algorithms. Each algorithm includes temperature dependence so that heating or annealing can be simulated. Simulation results include a plot of the energy of the cell per stage and a three-dimensional cell viewer with numerous features to aid the analysis and visualization of the computational cell at each of the stages (e.g., rotation and translation tools, show/hide by atomic species, layer, etc.), as shown in the following screen capture. An AVI movie file of the entire simulation process can be created and then viewed outside of *adwTools* on any computer or shared via Internet. Full connectivity between catalogs and simulations allows intermediate simulation stages to be used in a catalog or to launch a new simulation.



Currently adwTools performs two types of simulations: (1) Monte Carlo simulations based on the exchange of atoms of different species and (2) relaxation calculations where atoms vary their coordinates during the simulation according to different possible algorithms.

Long description. Monte Carlo simulation results in the left half of the screen show a graph of energies (chemical, strain, and total) versus simulation stage (temperature). The right half of the panel is an interactive three-dimensional representation of the computational cell at the simulation stage selected by the user on the energy graph.

Since its inception, *adwTools* has proven its versatility in a variety of applications, including the study of alloy surfaces, surface alloys, and bulk alloy design (refs. 2 and 3). Images and animations demonstrating the capabilities of the *adwTools* software can be found in the expanded online version of this article at http://www.icmsc.org/RT/

Find out more about this research:
International Computational Materials Science Consortium at
http://www.icmsc.org/
Glenn's Tribology & Surface Science Branch at
http://www.grc.nasa.gov/WWW/SurfSci/

References

1. Bozzolo, G., et al.: Surface Segregation in Multicomponent Systems: Modeling of Surface Alloys and Alloy Surfaces. Comput. Mater. Sci., vol. 15, no. 2, 1999, pp. 169-195.
2. Woodruff, D.P.: Surface Alloys and Alloy Surfaces. Elsevier, Amsterdam, 2002.
3. Wilson, A., et al.: Experimental Verification of the Theoretical Prediction of the Phase Structure of a Ni-Al-Ti-Cr-Cu Alloy. Acta Mater., vol. 50, no. 11, 2002, pp. 2787-2800.

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