

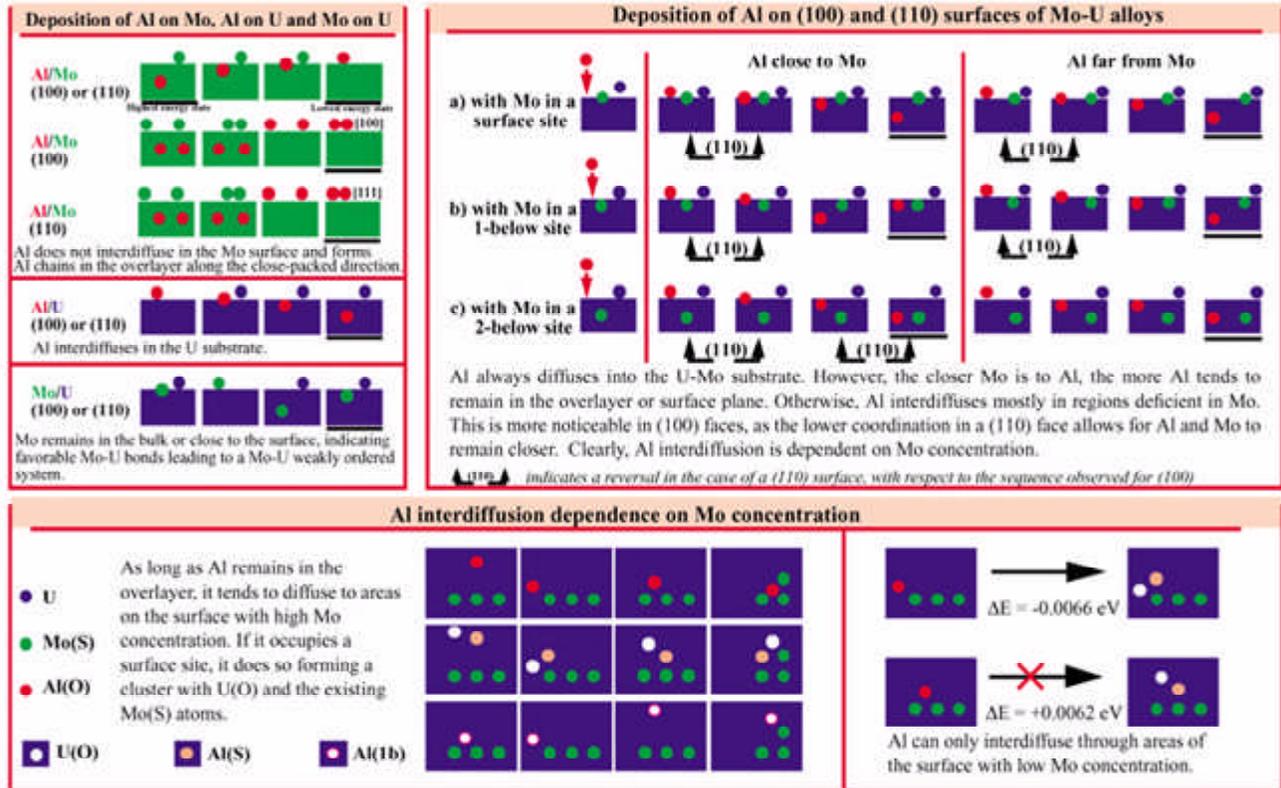
Alloy Interface Interdiffusion Modeled

With renewed interest in developing nuclear-powered deep space probes, attention will return to improving the metallurgical processing of potential nuclear fuels so that they remain dimensionally stable over the years required for a successful mission. Previous work on fuel alloys at the NASA Glenn Research Center was primarily empirical, with virtually no continuing research. Even when empirical studies are exacting, they often fail to provide enough insight to guide future research efforts. In addition, from a fundamental theoretical standpoint, the actinide metals (which include materials used for nuclear fuels) pose a severe challenge to modern electronic-structure theory. Recent advances in quantum approximate atomistic modeling, coupled with first-principles derivation of needed input parameters, can help researchers develop new alloys for nuclear propulsion.

Of particular relevance in these programs is the study of surfaces and interfaces, where engineered systems typically fail. Since the invention of scanning tunneling microscopy (STM) and the subsequent development of various scanning-probe-based techniques, unprecedented spatial resolution has been achieved using various surface probe methods, from near-field optical to scanning capacitance, even discrete I-V curves as a function of nanoposition. These surface analytic techniques have been fueled by and in turn fuel nanotechnology. In the study of surfaces, these relatively recent additions to a surface scientist's options join proven techniques for surface study such as small-spot auger electron spectrometry (AES), x-ray photoelectron spectroscopy (XPS), secondary ion mass spectrometry (SIMS), low energy electron diffraction (LEED) and others for the investigation of metallurgical problem areas. Interfacial analysis, even with the latest experimental tools, is a more challenging task because of the additional problem of extracting either the interface or information from a buried interface for analysis. The shortcomings of the experimental techniques available are most apparent in issues related to nuclear materials, where research is further limited by the focus on very specific applications, thus reducing the body of available data for these systems.

In recent years, the development of low-enrichment uranium fuel has been the main focus for many researchers. The development of high-density uranium (U) alloys with an increased concentration of U is one of the key prerequisites for developing high-neutron-flux research reactors with low enrichment uranium fuel (ref. 1). The uranium-molybdenum (U-Mo) alloy system is one of the prospective candidates because a solid solution of Mo in γ -U has acceptable irradiation properties for reactor fuels. The prospect of using a U-Mo alloy as a reactor fuel is closely connected with the possibility of retaining a metastable gamma-phase state in alloys at temperatures below 560 °C during fuel element fabrication and irradiation. The reactor fuel consists of atomized U-Mo particles in an aluminum matrix. An interdiffusion or interfacial reaction, which affects the performance of nuclear fuel materials, is observed in the U-Mo/aluminum (Al) composites for low Mo composition. The experimental results indicate a large volume change, 26 vol%, for U-2 wt% Mo/Al, mainly due to the formation of voids and cracks resulting from nearly complete interdiffusion or an interfacial reaction, with uranium aluminide formation. However, no significant dimensional changes are observed in the U-10 wt% Mo/Al

system. It is supposed that Mo atoms supersaturated in the grain boundary inhibit the diffusion of aluminum atoms (ref. 2). With such limited information, it is imperative to extend the scope of the tools used for the study of these issues, by including modeling techniques. In this article, we summarize results of an atomistic modeling description developed at the NASA Glenn Research Center of the main features observed experimentally in the diffusion of Al in the U-Mo solid solution. In what amounts to the first application of quantum approximate methods to nuclear materials, the ADW-SMP modeling package, which is based on the BFS (Bozzolo-Ferrante-Smith) method for alloys, was applied to the study of Al interdiffusion in U-Mo alloys.



Modeling results for the interdiffusion of Al in U-Mo alloys. The panel in the top left corner shows the binary cases, where one element (Al or Mo) is deposited on a single-element substrate (Mo or U) as a function of the crystal face ((100) or (110)). The panel in the top right corner displays the behavior of a deposited Al atom in a U-Mo alloy as a function of the surface orientation of the alloy and the closeness to Mo atoms in solution (representing regions of high or low Mo concentration in the alloy). The lower panel indicates that the interdiffusion of Al in the U-Mo substrate is the result of a series of energetically allowed transitions. In all cases, X(L) indicates an atom of species X (Al, U, or Mo) located in a surface site (S) or in the layer immediately above (O) or below (1b).

The preceding schematic displays a graphical description of the process of Al interdiffusion in U-Mo alloys. Several processes need to be included-the deposition of Al on Mo, Al on U, and Mo on U-to fully describe the contrasting behaviors that should be

taken into account when interpreting the results of the ternary case. The right panel in the schematic describes the intricate mechanism leading to the interdiffusion of Al in the U-Mo alloy, and the lower panel identifies allowed and prohibited processes that result in the observed behavior. In all panels, processes are depicted from left to right in terms of decreasing energy (i.e., increasing likelihood of occurrence). This level of understanding, for the first time available for this type of system, is fundamental when determining the steps necessary for modifying the system.

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