

Atomistic Method Applied to Computational Modeling of Surface Alloys

The formation of surface alloys is a growing research field that, in terms of the surface structure of multicomponent systems, defines the frontier both for experimental and theoretical techniques. Because of the impact that the formation of surface alloys has on surface properties, researchers need reliable methods to predict new surface alloys and to help interpret unknown structures. The structure of surface alloys and when, and even if, they form are largely unpredictable from the known properties of the participating elements. No unified theory or model to date can infer surface alloy structures from the constituents' properties or their bulk alloy characteristics. In spite of these severe limitations, a growing catalogue of such systems has been developed during the last decade, and only recently are global theories being advanced to fully understand the phenomenon.

None of the methods used in other areas of surface science can properly model even the already known cases. Aware of these limitations, the Computational Materials Group at the NASA Glenn Research Center at Lewis Field has developed a useful, computationally economical, and physically sound methodology to enable the systematic study of surface alloy formation in metals. This tool has been tested successfully on several known systems for which hard experimental evidence exists (refs. 1 and 2) and has been used to predict ternary surface alloy formation (results to be published: Garces, J.E.; Bozzolo, G.; and Mosca, H.: Atomistic Modeling of Pd/Cu(100) Surface Alloy Formation. *Surf. Sci.*, 2000 (in press); Mosca, H.; Garces J.E.; and Bozzolo, G.: Surface Ternary Alloys of (Cu,Au)/Ni(110). (Accepted for publication in *Surf. Sci.*, 2000.); and Garces, J.E.; Bozzolo, G.; Mosca, H.; and Abel, P.: A New Approach for Atomistic Modeling of Pd/Cu(110) Surface Alloy Formation. (Submitted to *Appl. Surf. Sci.*)). Ternary alloy formation is a field yet to be fully explored experimentally.

The computational tool, which is based on the BFS (Bozzolo, Ferrante, and Smith) method for the calculation of the energetics, consists of a small number of simple PC-based computer codes that deal with the different aspects of surface alloy formation. Two analysis modes are available within this package.

1. The first mode provides an atom-by-atom description of real and virtual stages during the process of surface alloying, based on the construction of catalogues of configurations where each configuration describes one possible atomic distribution. BFS analysis of this catalogue provides information on accessible states, possible ordering patterns, and details of island formation or film growth. More importantly, it provides insight into the evolution of the system. Software developed by the Computational Materials Group allows for the study of an arbitrary number of elements forming surface alloys, including an arbitrary number

of surface atomic layers.

2. The second mode involves large-scale temperature-dependent computer simulations that use the BFS method for the energetics and provide information on the dynamic processes during surface alloying. These simulations require the implementation of Monte-Carlo-based codes with high efficiency within current workstation environments.

This methodology capitalizes on the advantages of the BFS method: there are no restrictions on the number or type of elements or on the type of crystallographic structure considered. This removes any restrictions in the definition of the configuration catalogues used in the analytical calculations, thus allowing for the study of arbitrary ordering patterns, ultimately leading to the actual surface alloy structure. Moreover, the Monte Carlo numerical technique used for the large-scale simulations allows for a detailed visualization of the simulated process, the main advantage of this type of analysis being the ability to understand the underlying features that drive these processes. Because of the simplicity of the BFS method for the energetics used in these calculations, a detailed atom-by-atom analysis can be performed at any point in the simulation, providing necessary insight on the details of the process.

The main objective of this research program is to develop a tool to guide experimenters in understanding and interpreting often unexpected results in alloy formation experiments. By reducing the computational effort without losing physical accuracy, we expect that powerful simulation tools will be developed in the immediate future, which will allow material scientists to easily visualize and analyze processes at a level not achievable experimentally.

References

1. Bozzolo, G.; Ferrante, J.; and Ibanez-Meier, R.: Semi-Empirical Analysis of Surface Alloy Formation. Proceedings of the 1995 15th European Conference on Surface Science, vols. 352–354, 1996, p. 577–582.
2. Bozzolo, G., et al.: Surface Segregation in Multicomponent Systems: Modeling of Surface Alloys and Alloy Surfaces. *Comp. Mat. Sci.*, vol. 15, 1999, pp. 169–195.

Additional references are available via the World Wide Web.

http://www.grc.nasa.gov/WWW/SurfSci/bfs/bfs_index.html

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