Alloy Surface Science across Composition Space

Andrew J. Gellman
Dept. of Chemical Engineering, Carnegie Mellon University
Pittsburgh, PA 15213

Multicomponent materials are used throughout the energy, chemicals, electronics, manufacturing and many other industries. The critical value of multicomponent materials is that their properties are almost always superior to those of their pure components. Moreover, by selecting their composition appropriately multicomponent materials can be designed to optimize a number of functions simultaneously: e.g. catalytic activity, catalytic selectivity, corrosion resistance, mechanical properties, cost, … etc. One of the key challenges to systematic design and development of multicomponent alloys is the need to make, characterize, and test large numbers of samples each having a different composition. As an example, some steels contain 15 or more elemental components, each serving a different purpose and incorporated at specific concentrations, presumably identified to optimize performance. Identifying the overall composition is an experimental nightmare, especially when the different components interact with one another. We have addressed the experimental challenge associated with development of multicomponent materials by developing methods for preparation, characterization and property measurement on Composition Spread Alloy Films (CSAFs). These are thin alloy films deposited with lateral composition gradients such that an entire ternary composition space can be represented in a 1 cm^2 thin film; $A_xB_yC_{1-x-y}$, $x = 0 \rightarrow 1$, $y = 0 \rightarrow 1\text{-}x$. By using a suite of spatially resolved analytical tools, the alloy's physical characteristics (bulk composition, surface composition, electronic structure, phase, etc.) and its functional properties (catalytic activity, corrosion resistance, thermal conductivity, etc.) can be mapped rapidly across composition space (x, y). The presentation will cover some of the methods and then illustrate their application to catalysis on $Cu_xAu_yPd_{1-x-y}$ alloys and corrosion passivation of $Al_xFe_yNi_{1-x-y}$ alloys. These types of high-throughput methods offer the opportunity to accelerate materials discovery and optimization by factors of 10-100.