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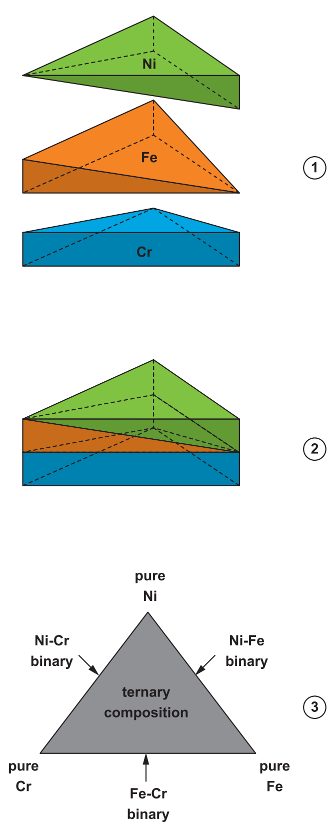
Development of Combinatorial Methods for Alloy Design and Optimization

New Tools and Techniques Demonstrate Combinatorial Design, Discovery, and Optimization of Alloys

Combinatorial materials science is a relatively new field that applies methods developed by the U.S. chemical and pharmaceutical industries for the rapid synthesis and evaluation of a large number of samples to the development of new engineering materials. Metal alloys are made by combining elements in varying ratios to produce a product that has unique physical properties such as strength, hardness, corrosion, and resistance. Small changes in the ratios of these elements can dramatically change physical properties.

Determining the optimal ratio of elements in multi-element systems could require manufacturing and testing hundreds of thousands of coupons. This project developed a comprehensive methodology for designing and optimizing metallic alloys using combinatorial principles. The basic concept was to develop techniques that can be used to fabricate an alloy specimen with a continuous distribution of binary and ternary alloy compositions across its surface - an "alloy library" - and then use spatially resolved probing techniques to characterize the structure, composition, and relevant properties of the library. Combinatorial methods promise to significantly reduce the time, energy, and expense needed for alloy design.



Schematic Diagram of the Alloy Library Coupon
Three controlled geometry thin film deposits are made and annealed to form one coupon with a continuous distribution of elements.

Benefits for Our Industry and Our Nation

A large number of alloy systems can be impacted by the new combinatorial technologies developed in this project. As proof-of-principle, the methodology was successfully applied to the ternary Fe-Ni-Cr system, which forms the basis of the commercially important H-series and C-series heat- and corrosion-resistant casting alloys.

This technology enables faster and less expensive alloy development. New alloys that can be used at higher operating temperatures result in higher industrial efficiencies, reduced energy use and less environmental impact.

Applications in Our Nation's Industry

Applications in which high-temperature alloys are used include: furnace fixtures; refiner fittings; boiler baffles; parts for cement/lime kilns and roaster furnaces; recuperators; coke oven exhausts; rolls; reformer, pyrolysis, and catalyst tubing; retorts; gas turbines; heat treatment fixtures and salt pots.
These materials have cross-cutting impacts in the following industries:

- Aluminum
- Chemical
- Forest Products
- Glass
- Heat Treating
- Metal casting
- Petrochemical
- Steel

Project Description

A new technique for high-intensity X-radiation structural and chemical characterization was developed. Nanoindentation techniques were used to investigate the elastic modulus and hardness of the libraries, and the resistance of the libraries to carburization and corrosion was tested. As proof of principle, the methodology was applied to the iron-nickel-chrome (Fe-Ni-Cr) ternary alloy system that constitutes the commercially important H-series and C-series heat- and corrosion-resistant casting alloys. Although this study was limited to one metallic system, the basic technique is applicable to a wide variety of alloys, and thus will lead to improved materials that crosscut the needs of many industries.

Barriers

Conventional techniques for alloy preparation consume considerable time, energy and expense, primarily because the methods are unavoidably restrictive in the range of alloy compositions that can be examined.

Pathways

The project pathway was to fabricate alloy specimens ("alloy libraries") with a continuous distribution of binary and ternary alloy compositions across its surface and then to use spatially resolved probing techniques to characterize structure, composition and other relevant properties. Specific objectives were to

- devise means by which test specimens with a library of alloy compositions could be produced,
- assess the properties of the combinatorially produced alloys vs. conventionally processed alloys, and
- devise screening tools to rapidly assess the important properties of alloys.

Results

Three different techniques were developed for making alloy libraries:

1. Vapor deposition of discrete thin films on a substrate, followed by solid-state diffusion of alloy film with the substrate.
2. Co-deposition of the alloying elements from three separate magnetron sputtering sources onto an inert substrate.
3. Localized melting of thin films with a focused electron-beam welding system.

A new technique for rapid structural and chemical characterization of alloy libraries based on high-intensity X-radiation from synchrotron sources was developed that allows for characterization of 2,500 positions in less than four hours. This methodology was applied to the Fe-Ni-Cr ternary alloy system.

Commercialization

Alloy compositions were chosen in consultation with industrial partners to establish alloys relevant to developing commercial products. This work was published in five papers in four journals between 2003 and 2005.

Project Reports

This project was completed in March 2005. The final report can be found on the Industrial Technologies Program Web site: http://www.eere.energy.gov/industry/imf/completed_rd.html

Project Partners

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A Strong Energy Portfolio for a Strong America

Energy efficiency and clean, renewable energy will mean a stronger economy, a cleaner environment, and greater energy independence for America. Working with a wide array of state, community, industry, and university partners, the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy invests in a diverse portfolio of energy technologies.

August 2006
Project completed in March 2005
CPS # 1778(Agreement #11205)