Development of Combinatorial Methods for Alloy Design and Optimization

Benefits

Although a large number of alloys will be impacted by the new combinatorial technologies developed in this project, as proof-of-principle the methodology will be first 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.

Among the anticipated benefits of new alloy compositions are

- Higher alloy use temperature with resulting higher industrial efficiencies in processes and environmental benefits.

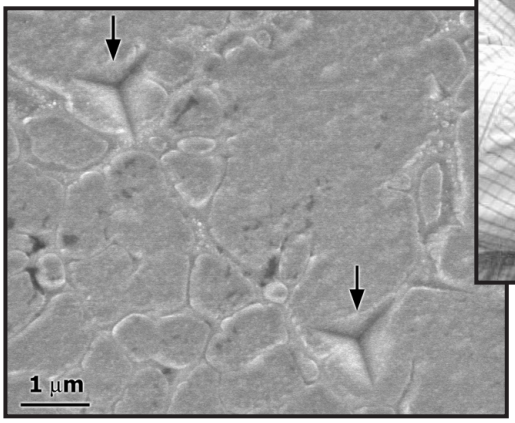
Applications

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

- **Chemical,**
- **Forest Products,**
- **Heat Treating,**
- **Metalcasting,**
- **Mining,**
- **Petrochemical,** and
- **Steel.**

Combinatorial methods for alloy optimization can significantly accelerate the development of new alloys with improved properties for use in IOFs

This project aims to develop a comprehensive methodology for designing and optimizing metallic alloys by combinatorial principles. Combinatorial methods promise to significantly reduce the time, energy, and expense needed for alloy design, largely because conventional techniques for preparing alloys are unavoidably restrictive in the range of alloy compositions that can be examined. The basic concept is to develop a technique 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. As proof of principle, the methodology will be applied to the Fe-Ni-Cr ternary alloy system that constitutes the commercially important H-series and C-series heat- and corrosion-resistant casting alloys. Combinatorial methods will also be developed to assess the resistance of these materials to carburization and aqueous corrosion, properties important in their application. Although the model study will be limited to one metallic system, it is envisioned that the basic techniques will be applicable to a wide variety of alloys and thus will lead to improved materials in a manner that crosscuts the needs of a large number of Industries of the Future.



Micrograph showing nanoindentations in an intermetallic alloy

Specimen being prepared for nanoindentation testing

Project Description

Goal: Develop a comprehensive methodology for designing and optimizing alloy systems by the use of combinatorial principles.

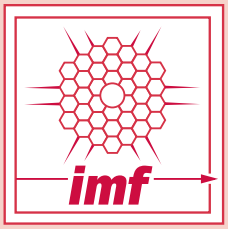
Issues: Conventional alloy design is cost prohibitive, especially for those applications where what is needed (rather than a brand new alloy) is the optimizing of an existing alloy composition to obtain improved properties. Combinatorial methodologies offer the promise of accelerating the entire process of alloy optimization at considerably reduced time and cost.

Approach: (1) Devise a means by which simple test specimens with a library of alloy compositions spanning the composition range of interest can be produced. (2) Assess how well the properties of the combinatorial specimens reproduce those of the conventionally processed alloys. (3) Devise screening tools that can be used to rapidly assess important alloy properties.

Potential payoff: Alloys with improved properties will allow more efficient and economical operation of processes throughout the whole range of Industries of the Future.

Progress and Milestones

- Production of binary and ternary alloy library test specimens.
- Assessment of combinatorial specimen quality.
- Mechanical property measurement by nanoindentation.
- Comparison with conventionally cast alloys.
- Assessment of carburization and corrosion resistance.
- High-speed structural characterization by micro-focus X-ray beams.
- Annual workshops to discuss progress with industrial partners.
- Quarterly and annual progress reports.



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Project Partners

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