



the **ENERGY** lab

## PROJECT FACTS

Advanced Research  
Materials

# Computational and Experimental Development of Novel High-Temperature Alloys

## Background

The need for fossil-fueled power plants to run cleaner and more efficiently leads toward ever-higher operating temperatures and pressures. Gas turbines, which can be fueled by natural gas, synthetic gas (syngas), or a high-hydrogen stream derived from coal, are critical components in this development. High-temperature operation of turbines is generally achieved by using nickel-chrome superalloys with coatings to improve thermal characteristics and resistance to oxidation and corrosion. The maximum temperature capability of current commercial coatings is limited to about 1,150 °C. Next-generation gas turbine technologies will require alloys that can function at about 1,350 °C in corrosive environments. Hence, design of ultra-high temperature alloys is a major task in gas turbine development.

To this end, the Department of Energy (DOE) National Technology Energy Laboratory (NETL) is partnering with Ames Laboratory to develop a method for finding novel materials capable of performing well at very high temperatures required by advanced coal-fired power systems. Further experimental screening will yield promising candidate alloys for further development.

## Project Description

This project will develop a tool to rapidly assess materials to find candidate high-temperature, oxidation-resistant alloys capable of meeting the requirements of high-temperature gas turbine components. The basis for this method is that materials can be compared using formation enthalpy data, which shows the heat released or absorbed in their formation. Using this tool will allow researchers to narrow down possible alloy formulations from tens of thousands to a manageable number of combinations that are most likely to succeed.

Project researchers will investigate potential alloy formulations using progressively more accurate thermodynamic methods; conduct critical experiments to test the accuracy of the calculations; and evaluate each alloy's key mechanical, thermal, and oxidation properties. Those alloys showing the greatest potential for high performance will be further screened for thermochemical stability using state-of-the-art thermal analysis, high temperature X-ray diffraction analysis, and microstructural evaluation with electron microscopy.

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## PROJECT DURATION

### Start Date

10/01/2007

### End Date

09/30/2011

## COST

### Total Project Value

\$355,000

### DOE/Non-DOE Share

\$355,000 / \$0

## NATIONAL ENERGY TECHNOLOGY LABORATORY

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## Goals and Objectives

The goal of this project is to develop high-temperature, oxidation-resistant alloys capable of meeting the requirements of high-temperature gas turbine components. Specific project objectives include (1) developing an extended Miedema model for a rapid estimation of formation enthalpies of multi-component alloys; (2) screening potential high-temperature alloys using the extended Miedema model, and conduct experimental studies on scale-forming ability of select alloys; (3) performing a more rigorous thermodynamic modeling of promising alloy systems, with the aims of tailoring alloy compositions and of feeding results back into the extended Miedema model; (4) developing databases, both experimentally and computationally, to supplement thermodynamic modeling; (5) conducting experimental studies on oxidation kinetics, microstructural characterization of oxide scale, and diffusion behavior of the tailored alloy compositions; and (6) conducting experimental studies on microstructure development.

## Accomplishments

The Miedema model has been extended to multicomponent alloys. Preliminary screening of potential alloys using the extended Miedema model resulted in rejection of alloys containing hafnium, yttrium, and zirconium as major components. Experimental studies on oxide scale resulted in identification of iridium as a good candidate for oxidation resistance.

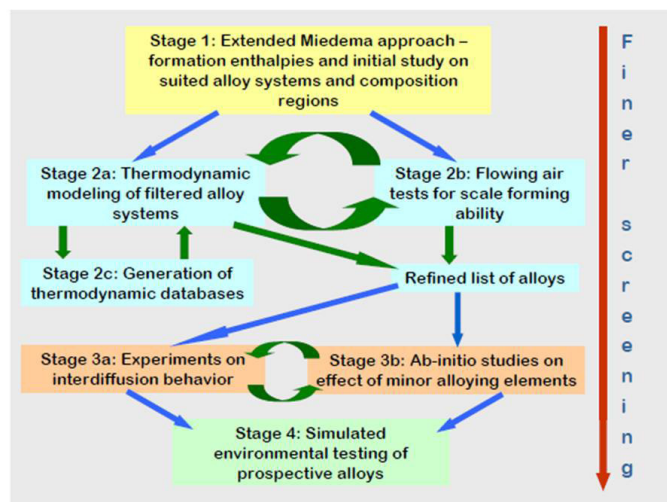


Figure 1. A schematic of the conceptual framework for the alloy development process.

Tests were conducted to determine the affect of alloy composition and preparation method on oxidation resistance. Alloy samples made by drop casting showed better oxidation resistance than alloy samples made by sintering. Nickel-aluminum-iridium alloys prepared with small additions of hafnium displayed the best oxidation resistance at 1,150–1,300 °C compared to other nickel-aluminum-platinum metal group alloy compositions that were tested.

## Benefits

The method developed by this project will improve the materials selection process for continued alloy design for the construction of components of advanced power systems. The alloys developed during this project for performance in high-temperature, high-pressure, corrosive environments will improve power plant operation. This will reduce emissions of greenhouse gases and pollutants for better environmental management. Higher process efficiencies will reduce costs and conserve energy resources.

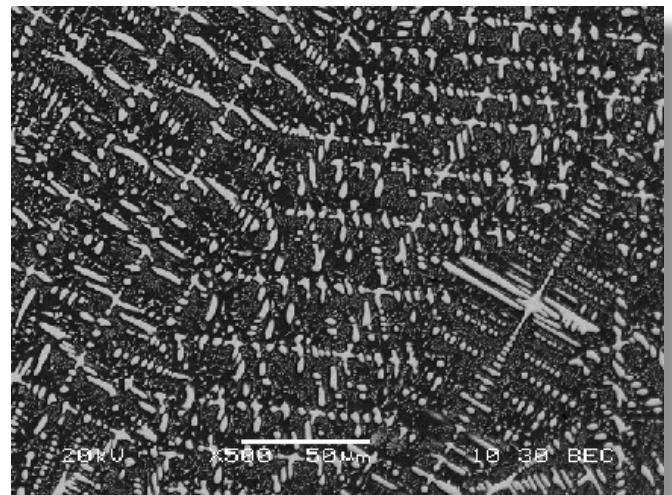


Figure 2. The micrograph of a selected alloy shows the skeleton-like framework required for good performance in these applications.

