the ENERGY lab

PROJECT FACTS

Advanced Research Materials

Computational Design of Materials

Background

The Department of Energy (DOE) aims to improve the efficiency and environmental performance of fossil power generation systems. New technologies such as advanced gas turbines and combustion systems are being designed to operate under more extreme conditions in order to achieve greater efficiencies and reduce emissions. Researchers at the National Energy Technology Laboratory (NETL) are developing alloys able to withstand the high temperatures, high pressures, and corrosive environments targeted for these advanced power plant components.

Alloys are formed by blending a metal with some other metallic or non-metallic elements to impart certain beneficial characteristics such as strength or heat and corrosion resistance. Alloys based on refractory metals – elements resistant to heat such as niobium (Nb), molybdenum (Mo), chromium (Cr), and tungsten (W) – are potential candidates. However, these alloys tend to exhibit low ductility (e.g., the ability of a material to be deformed plastically) and fracture toughness (the ability of a material containing a crack to resist fracture) at room temperature. Oxidation resistance and creep resistance, which indicate the tendency of materials to corrode and to deform at high temperatures, also need to be enhanced in order to develop these materials for use in advanced power systems. The two main difficulties in developing refractory alloys are (1) the lack of basic experimental data on thermodynamic, mechanical, and physical properties of most of these alloy systems, and (2) difficulties associated with processing these alloys for industrial use.

Theoretical modeling to guide experimental development reduces the need for time-consuming and expensive trial-and-error experiments to characterize these alloys. One approach to develop refractory metal-based alloys begins with integrated design, a computational method that facilitates materials development based on specific process and performance requirements. Integrated design utilizes multi-scale computational methods that predict material properties on a macroscopic level based on information or models from different (e.g., electronic, atomic, microstructural) levels.

Project Description

The NETL project team selected chromium to demonstrate the integrated design methodology for developing new high-temperature alloys based on refractory metals. Chromium was selected on the basis of its relatively low cost, relatively low density, and good high-temperature strength.

Researchers will perform theoretical studies using the integrated design approach to determine the structural, electronic, elastic, and thermodynamic properties of

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PARTNERS

None

PROJECT DURATION

Start Date
10/01/2009

End Date
09/30/2010

COST

Total Project Value
$399,998

DOE/Non-DOE Share
$399,998 / $0

Cr-based alloys and identify compositions that would have high ductility, melting point, and strength. The team will determine the effect of alloying elements on ductility. This will include theoretical studies to determine the effect of alloying elements on the Poisson's ratio – the ratio of the strain perpendicular to the applied load to the strain in the direction of the applied load – of Cr to identify compositions with a ratio of 0.33 or greater (implying intrinsic ductility).

To verify the computational results, researchers will perform experimental work including development of a series of Cr alloys on which to perform microstructural characterization at every stage of fabrication and mechanical testing to determine changes in ductility. The intrinsic ductility does not take into account the effects of defects (vacancies, impurities, dislocations, grain boundaries, second phase particles, etc.) in the structure. Although the real alloys always contain some finite concentration of a variety of defects, it is important to demonstrate that it is possible to improve ductility by manipulating bonds between atoms in Cr alloys. However, it is possible this improvement in ductility can be overwhelmed by extrinsic effect of defects. Commercial Cr and its alloys contain defects that interact with each other to alter mechanical properties of the alloy. Team members will investigate some of these extrinsic effects such as grain boundary segregation and dislocation mobility and manipulate them to improve ductility of Cr alloys.

Goals and Objectives

The two main goals of this project are: (1) to demonstrate that the synergistic integration of theoretical and experimental design can be used to develop new materials for high-temperature applications in energy systems, and (2) to improve the room temperature ductility of Cr-based alloys.

Accomplishments

Researchers studied the structural, electronic, elastic and thermodynamic properties of a variety of ternary and higher-order Cr-based alloys using first principle Density Functional Theory calculations. The goal was to identify compositions that are very ductile, that possess high melting point and high strength, and that contain coherent strengthening second-phase particles. The calculated Poisson's ratio values for various alloys are shown in Figure 1. Several compositions were predicted to have a Poisson's ratio of above 0.33, which suggests that they should be ductile. These compositions were recommended for experimental verification. In addition, 3D phase field simulations with poly-crystals and multiple orientations have been run successfully in the computer clusters. This simulation used 300 crystals and 200 randomly-selected orientations. The grain growth from tiny seeds to grains was shown. The grain boundary segregation phenomenon was revealed.

Researchers hot iso-statically pressed, homogenized, and extruded a series of Cr-V alloys and performed microstructural characterization using transmission electron microscopy, scanning electron microscopy, XRD, and microprobe at every stage of the fabrication. A mechanical testing program is in progress to determine ductility of these alloys. They also produced cast versions of these polycrystalline alloys using an arc melting technique. Specimens from the cast alloys were sent to Los Alamos National Laboratory (LANL) for determination of elastic properties using Resonant Ultrasound Spectroscopy (RUS). Ames Laboratory has grown single crystal samples so that the elastic properties of single crystal alloys can be measured.

Benefits

The integrated design modeling technique used by NETL researchers will provide greater insight into the structural behavior of Cr-based alloy systems under a variety of conditions. Successful development of a robust, inexpensive Cr-based alloy will help meet a key DOE NETL Materials Program objective to develop corrosion-resistant materials, particularly alloys, able to perform reliably at temperatures well over 1,000 °C. Project results will ultimately lead to new, more efficient, and environmentally sound fossil power generation systems that will increase U.S. energy output and security. This technique may also advance progress in other high-temperature areas such as aerospace applications, emission-control equipment, waste incineration, hot-working tools, petroleum refining, and petrochemical operations.

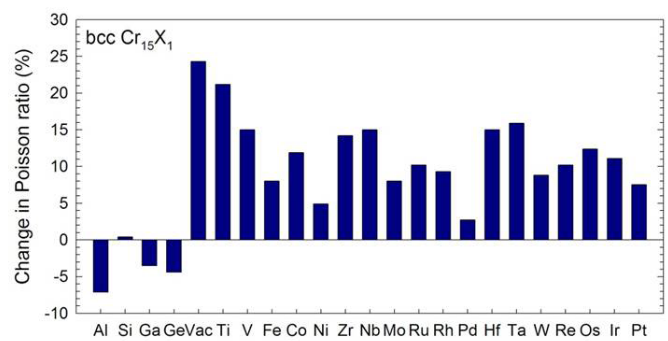

Figure 1. Effect of alloying elements (X) on the Poisson ratio of chromium as predicted by Density Functional Theory (DFT) calculations.

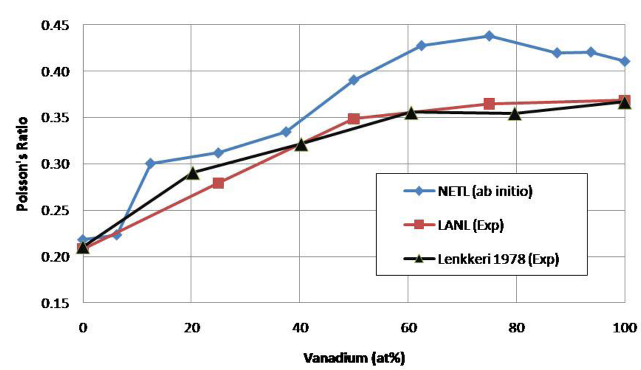

Figure 2. Variation in Poisson's ratio of chromium-vanadium (Cr-V) alloys as vanadium content changes. This graph shows a good correlation between the computational model results and the experimental results for this alloy.