the ENERGY lab

PROJECT FACTS

Advanced Research Materials

Computational and Experimental Design of Iron-Based Superalloys for Elevated Temperature Applications

Background

The Department of Energy's (DOE) Ultra-Supercritical Steam Boiler and Turbines Program calls for an increase of steam temperature, from 593 to 760 degrees Celsius (°C), by the year 2020. The National Energy Technology Laboratory (NETL) is sponsoring projects to improve the thermal efficiency of steam turbines by developing materials and processes which will allow these temperature increases. For this effort, NETL has selected the University of Tennessee at Knoxville to further develop a class of materials able to resist deformation under constant force at high temperatures, known as creep-resistant superalloys. These materials will be well-suited for applications in advanced power systems.

Project Description

This project will use a science-based systems-engineering approach to design advanced iron (Fe)-based superalloys capable of operating in the temperature range of 600 – 760 °C. The proposed research will employ modern computational tools for studies of phase stability, microstructure design, and coarsening dynamics. These analyses integrated with experimental results will provide a basis to guide alloy development.

The project will employ integrated first principles and computational-thermodynamic tools for the study of phase stability and microstructure design; perform nanoscale characterizations of fine microstructures; and conduct focused experiments to study creep behavior, ductility, and oxidation/corrosion resistance.

Goals and Objectives

The goals of this project are to design innovative superalloys for advanced fossil-energy systems operating at temperatures up to 760 °C and to create methods and tools that will form a framework for modern alloy design.

Project objectives include the further development of a new high-temperature, creep-resistant class of ferritic "superalloy" steels for applications in advanced steam-turbine systems; the establishment of robust, validated databases for the high-temperature alloy design process; and demonstration of a computation-based, systems engineering approach for designing advanced Fe-based superalloys by

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PARTNERS

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PROJECT DURATION

Start Date
01/15/2009

End Date
01/14/2012

COST

Total Project Value
$442,818

DOE/Non-DOE Share
$300,000 / $142,818

integrating a hierarchy of computational tools. A further expected outcome is the training of doctoral students in the integration of state-of-the-art computational and experimental methods that will become a framework for alloy design.

Accomplishments

Researchers identified a composition with ideal characteristics for a detailed analysis. Samples were prepared and tested using atom-probe tomography (APT) to investigate the microstructure and partitioning behaviors of the alloying elements. Additional tests showed improved creep resistance of this alloy composition.

Researchers developed mathematical models to predict the crystal lattice parameters of given phase compositions of the Fe-Ni-Cr-Al alloys tested in this project. Additional creep/strain tests were conducted on one of the experimental alloy composition, and creep modeling/mechanism work was performed on these test data.

Benefits

The superalloys developed from this research will provide materials capable of operating at the elevated temperatures targeted by the DOE to achieve by 2020. The processes created during their development will provide tools with which to design other materials of this type. The use of these materials and design tools will enable a new generation of higher-efficiency steam turbines, leading to reduced emissions of greenhouse gases, lower-cost power generation, improved resource conservation, and reduced reliance on foreign sources of energy.

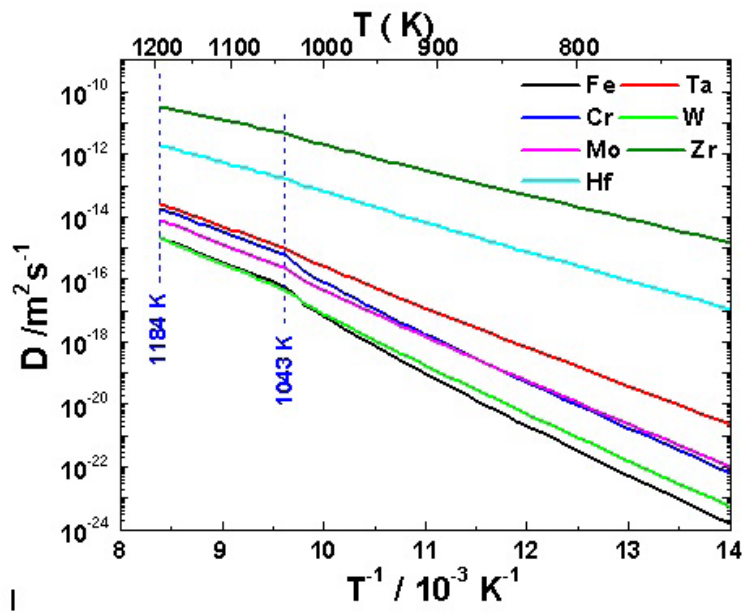
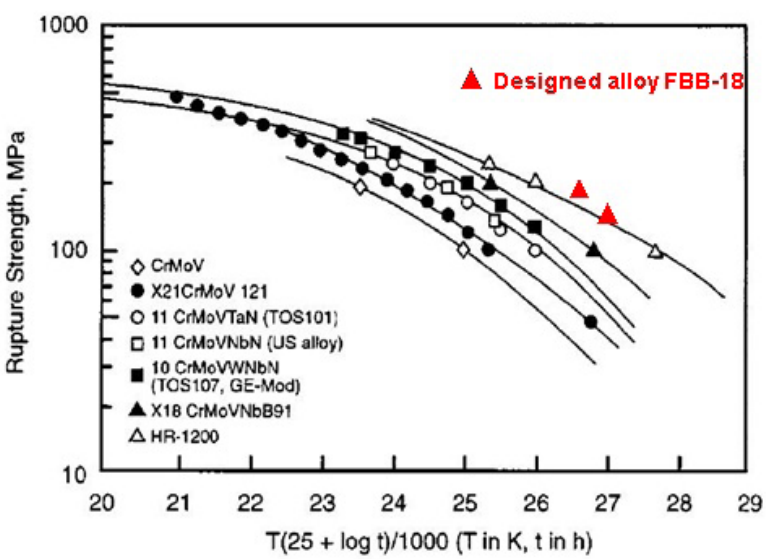


Figure 1. Predicted temperature dependence of the diffusion coefficients for the metals W, Mo, Ta, Cr, Zr, and Hf in α-Fe, compared with that for self-diffusion of Iron (Fe) in α-Fe. The diffusion coefficients are determined by first-principles calculations.



A comparison of the rupture strength between one of the designed alloys, FBB-18, and other candidate ferrite-based materials for steam-turbine applications. Creep rupture strength is a function of time and temperature. The creep resistance of FBB-18 at applied stresses of 140 MPa (20376 psi) and 170 MPa (24743 psi) is greater than the other candidate materials shown on the graph.