PROJECT facts

U.S. DEPARTMENT OF ENERGY
OFFICE OF FOSSIL ENERGY
NATIONAL ENERGY TECHNOLOGY LABORATORY

Advanced Research

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COMPUTATIONAL DESIGN OF FERRITIC-ALUMINA-STRENGTHENED ALLOYS

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Description

Innovative, high-temperature, corrosion-resistant materials are critical to improving efficiency and lowering emissions of advanced turbine power generation systems — key elements in the development of new coal-based energy systems. Through its University Coal Research (UCR) Program, the U.S. Department of Energy (DOE) Office of Fossil Energy (FE) is funding joint research among the University of Tennessee at Knoxville, Northwestern University, and the University of California, Davis (UCD), to develop a new class of "superalloy" steels for use in advanced coal-based energy systems. The research is advancing the development of computational models used to accelerate the design of high-temperature ferritic steel materials.

This project entails the use of a computer-aided alloy design approach to optimize the development of high-temperature materials through: (1) utilizing high-performance computations and simulations to identify prototype alloy compositions and heat treatments; and (2) employing a wide range of experimental techniques to synthesize, characterize, and gauge the properties of the prototype alloys. Northwestern and UCD will collaborate in conducting the fundamental — known as "first-principles quantum-mechanical" — calculations to develop reliable multicomponent thermodynamic and kinetic databases for the alloy design effort.

First-principles quantum-mechanical calculations: Term used in computational quantum chemistry to refer to use of high-performance computing power to predict the cohesive properties of moecules and compounds based on approximate solutions of the many-electron Schrödinger equation.

The University of Tennessee will lead the efforts in alloy fabrication, mechanical property studies, and oxidation/corrosion investigations. Both Northwestern and the University of Tennessee will also collaborate in microstructural characterizations using, for example, scanning electron microscopy (SEM), conventional transmission electron microscopy (TEM), high-resolution transmission electron microscopy (HR-TEM), and X-ray diffraction (XRD).

Objective

The objective of the research is to demonstrate the efficacy of modern computational tools in designing innovative ferritic super alloys strengthened mainly by nickel-aluminum (NiAl) -type precipitates for fossil energy applications up to 760 °C (1,033 K). A desirable Fe-based alloy would possess relatively high volume fractions

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PROJECT DURATION

03/06/06 to 04/30/09

COST

Total Project Value
$660,193

DOE/Non-DOE Share
$399,794 / $269,399

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of thermodynamically stable and coherent nanoscale precipitates with the cubic *B2* (NiAl-type) and/or $L2_1$ (Ni_2TiAl-type) structures. The research will employ modern computational tools for the study of phase stability, microstructure design, and coarsening dynamics, all of which will permit rapid exploration of new materials for these applications. This approach will be the basis for developing prototype ferritic super alloys having: (1) a steady-state creep rate of approximately 10^{-11} s^{-1} at 1,033 K and a stress level of 35 Mega pascals (MPa), (2) good low-temperature ductility, and (3) oxidation/corrosion resistance at elevated temperatures.

Technical Approach

A hierarchy of computational and experimental tools will be used to design and evaluate prototype alloys. Modern computational tools will be employed for the phase-stability study and microstructure design. Computational thermodynamic and kinetic programs, including Thermo-Calc and DICTRA software systems, will be used to integrate the design and process modeling of the proposed Fe-based alloys. Comprehensive first-principles-based calculations will be performed to predict the phase stability of all equilibrium phases in the Fe-Al-Cr-Ni system and to quantify the phase separation between the disordered *A2* (i.e., a body-centered cubic [bcc] Fe-based solid solution) and ordered *B2* (i.e., NiAl-type structures) phases.

A comprehensive mobility database for the equilibrium phases will be developed to simulate the kinetics of diffusional transformations. Calculations of impurity diffusion constants in the dilute limit will be developed in the search of slow-diffusing elements to be used to improve the coarsening resistance of precipitate phases in ferritic-superalloy microstructures. Incorporating the capillarity and the effective strain energy of a two-phase coherent mixture in computational thermodynamic and kinetic models will allow the prediction of the composition trajectory and coarsening process of nanoscale precipitates in multicomponent Fe-based alloys.

Predicted microstructures will be verified by fabricating the designed alloys and performing microstructural characterizations using TEM, HR-TEM, and XRD. Iron-based alloys will be sought that give a relatively high volume fraction of thermodynamically stable and coherent nanoscale precipitates. These alloys will be evaluated for their creep rates and oxidation/corrosion resistances in superheated steam with respect to the design target, which will provide important feedback to confirm the alloy design process.

Outcomes

Anticipated outcomes of the present work include: (1) development of a new high-temperature, creep-resistant class of ferritic superalloy steels for applications in advanced, coal-based energy systems; (2) establishment of robust, validated databases for the accelerated development and evaluation of elevated-temperature alloy designs; and (3) dissemination of research results through available channels.

Reference:

1. J. Philibert, Atom Movements: *Diffusion and Mass Transport in Solids* (*Les Editions de Physique, 1991*).