PROJECT facts

Advanced Research

08/2007

U.S. Department of Energy
Office of Fossil Energy
National Energy Technology Laboratory

Computer-Aided Design of Materials for High-Temperature Operating Conditions

Description

Through its University Coal Research (UCR) Program, the U.S. Department of Energy (DOE) Office of Fossil Energy (FE) is funding a three-year research project directed by the National Energy Technology Laboratory (NETL) and performed by Texas A&M University to develop a computational methodology to aid in the design of a wide variety of high-temperature materials for use in advanced coal-based energy systems. New materials are required to improve performance and reduce costs of existing power systems. They also are needed to develop new, more efficient, and environmentally acceptable systems for coal combustion and gasification, gas separation, hydrogen storage, high-temperature fuel cells, and advanced turbine systems.

The empirical methods currently used to optimize production and performance of advanced materials require long development cycles, considerable expense, and a great deal of trial and error to determine creep characteristics, oxidation resistance, elevation of melting point, thermal and electrical conductivity, and other thermal and electrical properties. This project will investigate the use of advanced computational methods to accelerate the design of such materials, thereby minimizing experimentation time. The methodology will be targeted toward single-crystal turbine blades, the subject of previous research on superalloys performed by Texas A&M (also directed by NETL), although the approach can be used for a variety of other materials as well.

Objectives and Technical Approach

The primary objective of this research is to develop a computational-based optimization method to aid in the design and development of materials operating at high temperatures. Supporting objectives and tasks include the following:

1) Develop a robust thermodynamic framework that can describe the continuum-level response of the class of materials that are being fashioned to the microstructure of the material itself. This framework will incorporate the variety of microstructural features, such as dislocation density, lattice mismatch, stacking faults, volume fractions of inclusions, and interfacial area, based on the choice of appropriate thermodynamic functions for the stored energy and the rate of heat transformation (entropy production). Resulting models then will be used to study the response of the materials under various conditions of heat and stress by solving typical initial- and boundary-value problems using differential equations.

2) Develop computational tools, through user-defined material sub-routines (known as UMATs), to utilize the models developed in comprehensive finite element software. ABAQUS is the selected computational tool, which is a robust software specifically designed for solving nonlinear problems related to heat and stress. The material models developed through this project will interface with ABAQUS,

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PROJECT DURATION

02/07/06 to 02/09/09

COST

Total Project Value
$199,866

DOE/Non-DOE Share
$199,866 / $0

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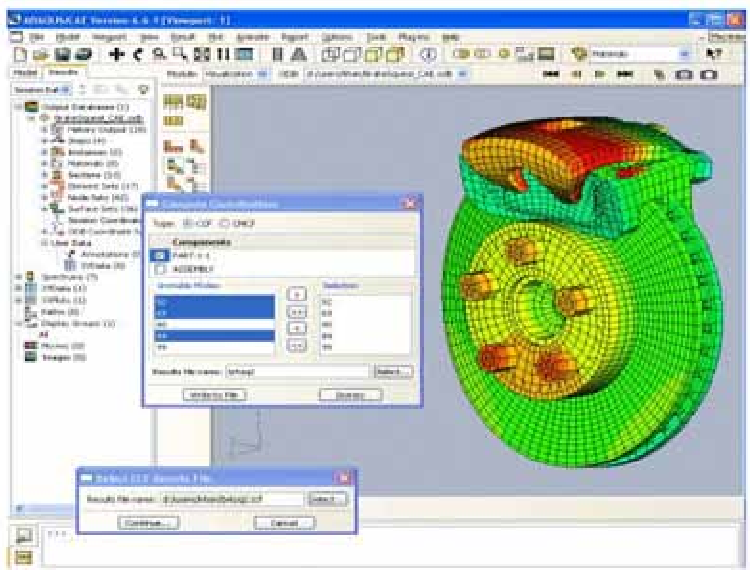
through UMATs to be developed as part of the research. Predictions from ABAQUS will be compared to known results and to results obtained from other numerical methods, and will be used to verify the accuracy of the numerical scheme employed.

3) Based on a set of desired response characteristics to be used as the benchmark, develop an interactive program that will optimize alternatives for stored energy, rate of entropy production, and other factors to be considered in determining how the material should be engineered. Using the ABAQUS software, this interactive optimization scheme will connect the models with the desired outcomes, so models can be systematically varied and their efficacy tested with respect to a desired response.



ABAQUS modeling software aids in complex problem solving, as in this bolt design problem

The basic tools developed in the prior tasks will be used to optimize the material's design by varying choices of the different thermodynamic functions, consistent with variations in the microstructure of the material. This iterative method will be carried out in a way to maximize or minimize the desired response. Connections between the thermodynamic functions (i.e., the microstructure) and the desired property will be clarified by investigating a large number of cases computationally.

Summary of Expected Outcomes

Year 1: Development of models that connect microstructure to continuum response and preliminary implementation in ABAQUS.

Year 2: Refinement of models and development of UMATs to incorporate into ABAQUS; testing the implementation and verifying its accuracy by comparison against known experimental data.

Year 3: Implementation of optimization methodology to either minimize unwanted characteristics or maximize desired characteristics such as creep life.

Benefits

Successful performance of this research will result in the ability to efficiently design and engineer related materials, which will lead to enhanced performance of the materials, significant cost savings, and a reduction in the time necessary to produce such materials. One important application with potential significant savings is the development of advanced turbine blades for a variety of applications, including power generation and aircraft engines.