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PROJECT FACTS

Hydrogen Turbines

Computational Design and Experimental Validation of New Thermal Barrier Systems—Louisiana State University

Background

Thermal barrier coating (TBC) systems safeguard modern gas turbine engines against significant temperature extremes and degradation. In order to develop reliable gas turbine power systems operating on coal-derived synthesis gas (syngas), such as integrated gasification combined cycle (IGCC) plants, robust TBCs must be developed to overcome material degradations from corrosion, erosion, and deposition due to the usage of high-hydrogen-content syngas. With current theoretical simulation tools and computer hardware power, material static and dynamic properties can only be investigated on very small scales (nano-size or smaller), and thus are not adequate for complicated high performance TBC design. Researchers from Louisiana State University (LSU) and Southern University (SU) are working on the development and evaluation of a computational materials tool using unique calculation schemes for the identification of new TBCs for harsh IGCC environments.

This project was competitively selected under the University Turbine Systems Research (UTSR) Program that permits academic research and student fellowships between participating universities and gas turbine manufacturers. Both are managed by the U.S. Department of Energy (DOE) National Energy Technology Laboratory (NETL). NETL is researching advanced turbine technology with the goal of producing reliable, affordable, and environmentally friendly electric power in response to the nation's increasing energy challenges. With the Hydrogen Turbine Program, NETL is leading the research, development, and demonstration of these technologies to achieve power production from high hydrogen content fuels derived from coal that is clean, efficient, and cost-effective, minimizes carbon dioxide (CO_2) emissions, and will help maintain the nation's leadership in the export of gas turbine equipment.

Project Description

New TBC materials can be tested for mechanical, physical, and chemical properties by altering the bond coat and top coat compositions. Current studies on TBCs are usually performed by trial-and-error approach. As the trial-and-error process is usually very expensive and time consuming, the LSU/SU team proposes to design a high performance TBC with enhanced top and bond coat through a reliable and efficient theoretical/computational approach. This can be used systematically to identify promising TBC bond coat and top coat compositions. Using high performance computing (HPC) simulations, an *ab initio* (i.e., from first principles) molecular dynamics (MD)-based design tool can screen and identify TBC systems with desired

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PROJECT DURATION

Start Date	End Date
10/01/2010	09/30/2014

COST

Total Project Value
$634,671

DOE/Non-DOE Share
$504,863/$129,808

AWARD NUMBER

FE0004734

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physical properties. Such computations work from basic or fundamental laws of nature to derive effects without intervening assumptions or special models, in principle producing well-founded results. The new TBC systems will be demonstrated experimentally under IGCC environments.

Goals and Objectives

The goal of this project is to develop and evaluate a novel TBC design tool based on the integration of *ab initio* density functional theory (DFT) with classical molecular dynamics method. Project objectives are as follows:

- Implement an integrative approach of *ab initio* calculations with molecular dynamics simulation and to develop the required computer code.
- Perform *ab initio* MD simulations using HPC to identify the most promising TBC compositions.
- Perform experimental validations on the promising TBC systems identified in the computational simulations.

Accomplishments

- The UBER (universal binding energy relation) relation-fitting code with Council of European Nuclear Research (CERN) library has been tested.
- Performed *ab initio* DFT simulation on the chromium (Cr), cobalt (Co), and yttrium (Y) crystals. The simulated lattice constant, bulk modulus, and magnetic moment are in good agreement with corresponding experimental results.
- The materials design environment MedeA® was implemented in HPC lab and tested with Cr and Y crystals.
- The concentration of aluminum (Al) in ternary AlxTaIr (tantalum iridium) is between 2.7 and 5.5 atomic percent and extra dopant type may be needed to coordinate with other three component elements (Figure 1).
- Design and fabrication of the TBC durability testing rig has been completed.
- Thermal cycling tests on TBC samples for gadolinium zirconate/yttria-stabilized zirconia (GZ/YSZ, GZ50%/YSZ etc.) have been conducted (Figure 2).
- Hot corrosion tests on YSZ-Ta_2O_5 top coats have been performed (Figure 3).

Benefits

This UTSR project supports DOE's Hydrogen Turbine Program that is striving to show that gas turbines can operate on coal-based hydrogen fuels, increase combined cycle efficiency by three to five percentage points over baseline, and reduce emissions. The TBC design tool and optimized high performance TBCs will play an important role in the development of next generation gas turbine engines. As no computational materials-based TBC design tool is currently available for advanced TBC design, this project makes significant contributions to the technical goals of the Hydrogen Turbine Program for developing advanced turbine materials.

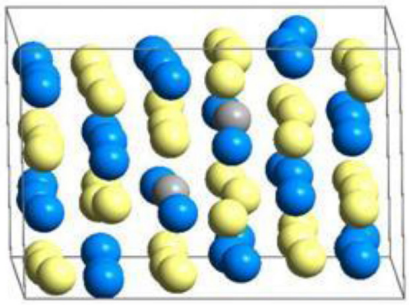

Figure 1. The 2Al-34Ta-36Ir crystal structure model used in one of our simulations. The gray balls are Al atoms, blue balls are Ta atoms, and yellow balls are Ir atoms. The two Ta atoms are substituted by two Al atoms.

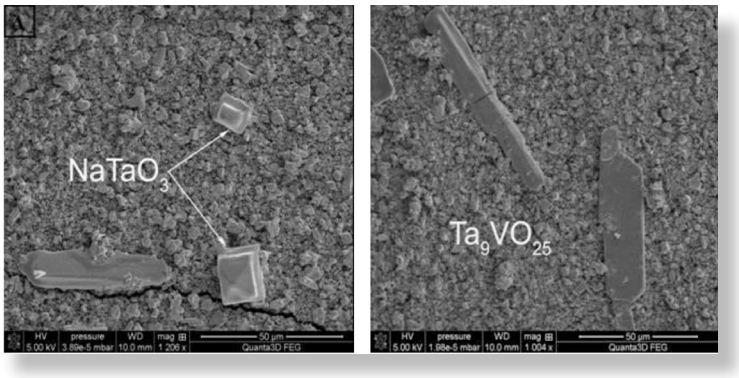

Figure 3. SEM surface images of TaYSZ after hot corrosion in $Na_2SO_4 + V_2O_5$ at 1100 °C.

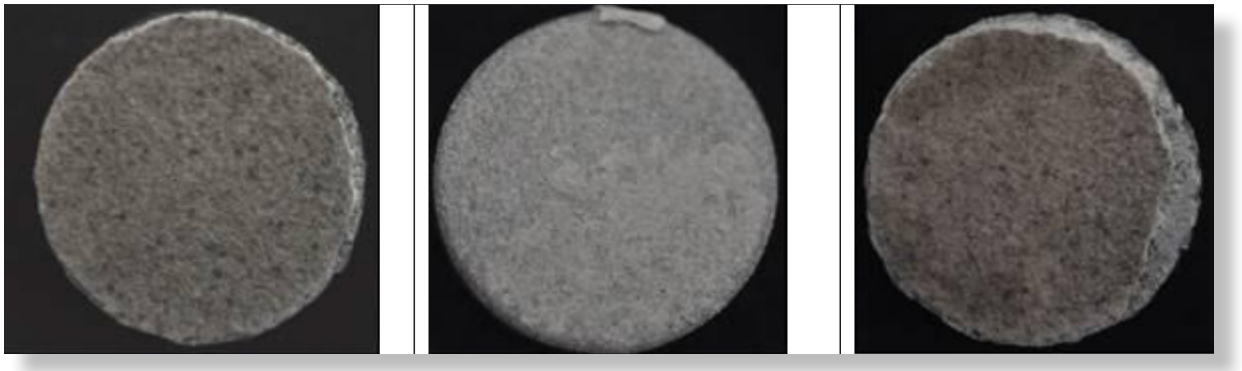

Figure 2. (L) YSZ, (M) GZ, (R) 50%GZ/YSZ, Failed TBC samples after thermal gradient thermal cycling tests. Failure is mainly caused by the spallation at the edges.