the ENERGY lab

PROJECT FACTS

Advanced Research

Multiscale Modeling of Grain Boundary Segregation and Embrittlement in Tungsten for Mechanistic Design of Alloys for Coal Fired Plants

Background

The Department of Energy (DOE) National Energy Technology Laboratory (NETL) University Coal Research (UCR) Program seeks to further develop the understanding of coal utilization. Since the program's inception in 1979, its primary objectives have been to improve our understanding of the chemical and physical processes involved in the conversion and utilization of coal in an environmentally acceptable manner; maintain and upgrade the coal research capabilities and facilities of U.S. colleges and universities; and support the education of students in the area of coal science.

As part of the UCR Program, NETL has partnered with Clemson University and Purdue University in a project that will predict grain boundary segregation and embrittlement of alloys to be used in coal-fired plants. The anticipated impact of the project is significant as it will accelerate the development of new materials that can enable efficiency improvements in fossil fuel systems while reducing carbon dioxide (CO_2) emissions.

Project Description

This project will investigate grain boundary segregation and embrittlement in modeled systems. The modeled systems for this project will be nickel (Ni) doped tungsten (W) and Ni+X co-doped [where X = copper (Cu), cobalt (Co), iron (Fe), palladium (Pd), carbon (C), and sulfur (S)]. Project personnel will then develop thermodynamic theories and statistical models to compute the grain boundary diagrams of the model systems. The developed models will link grain boundary segregation with grain boundary embrittlement. The models will be validated by experiments conducted by the researchers.

Specifically, multiscale modeling and simulation will combine quantum mechanics and atomistic hybrid Monte Carlo methods to calculate key thermodynamic properties. The results will be incorporated in cohesive finite

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PARTNERS

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PROJECT DURATION

Start Date
07/01/2010

End Date
6/30/2013

COST

Total Project Value
$328,196

DOE/Non-DOE Share
$300,000 / $28,196

element method (CFEM) fracture simulations to predict the effects of grain boundaries on properties and in CFEM analyses of fracture failure of refractory alloys that consider microstructures and grain boundaries.

Goals and Objectives

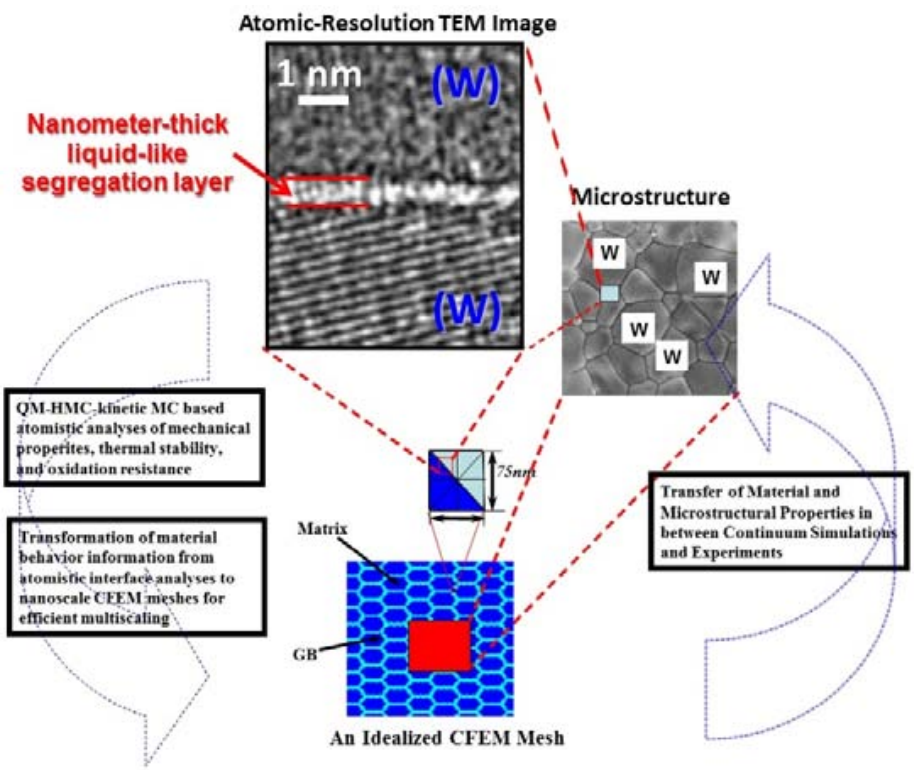
The project will develop a quantitative model for predicting grain boundary segregation in refractory alloys. Researchers will utilize this model to develop a multiscale modeling strategy to predict grain boundary embrittlement from grain boundary segregation.

To achieve this goal, the project will complete the following objectives:

- Develop thermodynamic models and quantitative grain boundary diagrams for predicting high-temperature grain boundary segregation and disordering in multi-component refractory alloys.
- Develop multiscale modeling strategies to predict grain boundary embrittlement from grain boundary structures and chemistry.
- Identify criteria for selecting co-dopants to alleviate grain boundary embrittlement.
- Develop strategies to remediate grain boundary embrittlement and control oxidation resistance.

Benefits

NETL is developing a technology base for the construction of the highly efficient, near-zero-emissions power plants of tomorrow. This project will make progress toward providing improved materials and modeling of these materials to allow for implementation in fossil energy conversion technologies. With enhanced understanding of grain boundary segregation and grain boundary embrittlement of refractory alloys, a higher standard of fossil energy conversion can be achieved.



A pictorial representation of the multiscale modeling approach *Source: Jian Luo*