the ENERGY lab

PROJECT FACTS

Advanced Research Materials

Computational Modeling and Assessment of Nanocoating for Ultra-Supercritical Boilers

Background

In order to improve the efficiency and environmental performance of fossil power generation systems, new technologies are being developed to meet the Department of Energy's (DOE's) goal of generating power using advanced steam cycles in boilers at ultra-supercritical (USC) conditions—operating temperatures to 760 degrees Celsius (°C) and pressures to 35 megapascals (MPa). USC conditions may increase efficiency up to 60 percent and decrease carbon dioxide and other fuel-related emissions in coal-based power plants. These advanced USC boilers require materials that can withstand high temperatures and pressures in corrosive environments.

Steels and other alloys have been developed to withstand high-temperature conditions, but specialized coatings are often needed to improve resistance to thermal creep (deformation at high temperatures) and corrosion. Metal alloy coatings consisting of elements such as iron (Fe), nickel (Ni), aluminum (Al), chromium (Cr), yttrium (Y), and cobalt (Co) have the potential to impart exceptional hardness as well as temperature and corrosion resistance to components for the next generation of USC coal-fired boilers. How well these nanostructured coatings impart the desired characteristics depends on a variety of factors such as the type and amounts of the various elements in the alloy system, the ability of the alloy coating to bond to the underlying substrate, and the quality of the coating process.

Project Description

The DOE National Energy Technology Laboratory (NETL) is partnering with Electric Power Research Institute (EPRI), with support from Southwest Research Institute (SWRI), Foster Wheeler, and Applied Materials, to use science-based computational methods to select the chemical composition of candidate nanocoatings, develop advanced coating application processes for depositing nanostructured coatings, and validate coating performance through laboratory-scale tests in simulated boiler environments.

Potential nanostructured coating compositions will be selected through (1) computational simulation software to develop phase diagrams; (2) a grain growth model to examine nanostructure phase stability; and (3) a fracture mechanics-based model to predict the tensile ductility (the ability of a material to be stretched, e.g., into a wire), fracture toughness (the ability to contain a crack and resist fracture),

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PARTNERS

Southwest Research Institute
Foster Wheeler
Applied Materials

PROJECT DURATION

Start Date
08/14/2007

End Date
06/21/2011

COST

Total Project Value
$2,493,536

DOE/Non-DOE Share
$1,994,828 / $498,708

and interface toughness of these coatings. Researchers will perform accelerated laboratory testing on the conventional and nanostructured coated specimens, and will characterize the exposed specimens to assess the extent of corrosion attack.

Other aspects to be investigated include validation of the phases predicted for selected alloy compositions, evaluation of heat transfer characteristics of each coating/alloy substrate combination, development of a coating life model, and evaluation of the thermal performance of coated boiler tubes.

Goals and Objectives

The goal of this project is to improve the reliability and availability of fossil-fired USC boilers and oxy-fuel combustor demonstrate nanostructured coatings through computational modeling methods that will significantly improve corrosion and erosion performance of tubing used in USC boiler applications.

Accomplishments

Phase diagrams were developed using ThermoCalc modeling software for a variety of coating systems. Specific chemistries were established where the appropriate phases would be present. These computational results were compared to, and agreed with, experimental results. The iron-chromium-nickel-aluminum (Fe-Cr-Ni-Al) alloy coating system was selected for use in the computational modeling phase of the project. Two specific nanocoating compositions were selected as candidate coatings. Both form a barrier layer at the interface between the coating and the substrate that reduces inward diffusion, thereby improving corrosion protection. Precise deposition parameters (amperage, voltage, coating thickness, deposition times, grain size, and aluminum percent) were established for two coating/substrate combinations using a plasma enhanced magnetron sputter (PEMS) technique.

Three substrate materials were selected for deposition evaluations and nanocoatings were applied to the substrate materials resulting in a matrix of 17 coating/substrate combinations. Metallurgical characteristics of each combination were analyzed to determine coating uniformity, density, grain size, thickness and bonding ability. The results of metallographic and cyclic oxidation testing showed that two interlayer ceramic materials are acceptable barrier coatings to minimize diffusion of elements from the top nanocoating into the substrate. Coatings were applied and testing started on advanced nanocoatings. These coated samples were exposed to 1464 each one-hour thermal cycles. Results of examinations by optical microscopy and scanning electron microscopy (SEM) showed that none of the three coatings exhibited evidence of oxidation. Switching from a two (2) magnetron to a larger four (4) magnetron coating deposition system resulted in nanocoatings that were free from cracks. Four (4) nanocoating compositions showed good resistance to sulfidation attack up to 818 °C in lab scale tests.

Benefits

This project will enhance U.S. energy security by identifying and developing advanced nanostructured coatings that will make it possible to maintain a cost-competitive, environmentally acceptable, coal-based electric generation option, as well as enable domestic boiler manufacturers to successfully produce and sell high-efficiency, coal-fired power plants in the global marketplace.

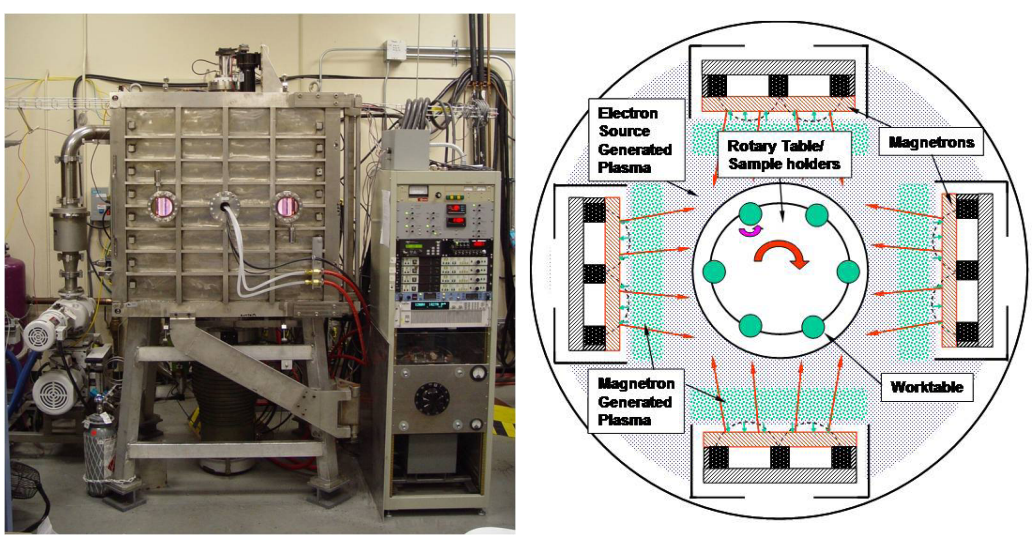

Figure 1. Photo and schematic of Plasma Enhanced Magnetron Sputtering (PEMS) Chamber, one cubic meter cube with four magnetrons.Chamber, one cubic meter cube with four magnetrons.