PROJECT facts

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

Advanced Research

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DUCTILITY ENHANCEMENT OF MOLYBDENUM PHASE BY NANO-SIZED OXIDE DISPERSIONS

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Description

Using computational modeling techniques, this research aims to develop predictive capabilities to facilitate the design and optimization of molybdenum (Mo), chromium (Cr), and other high-temperature structural materials to enable these materials to withstand the harsh environments of advanced power generation systems, such as gasification-based systems. These types of materials are essential to the development of highly efficient, clean energy technologies such as low-emission power systems that use coal or other fossil fuels.

Recent advances in the field of nanotechnology have made it possible to fabricate and stabilize nano-sized ceramic dispersions in metal solids. Since only atoms near the surface/interface layers are engaged in mechanisms to enhance ductility (malleability, or ability to be molded or shaped without breaking), nano-sized particles are expected to be more active due to their higher ratio of surface-to-bulk atom numbers. In addition, nanoparticles are easier candidates for surface or interface reconstructions, which may help reduce local stress and detrimental effects caused by the mismatch of mechanical properties between the ceramic and metal phases. These properties make nanoparticles particularly desirable as dispersion materials, especially high-temperature alloys such as those in the molybdenum-silicon (Mo-Si) system.

A number of Mo-based structural materials are being developed for ultra-high-temperature (greater than 1,000 ºC) applications beyond those presently attainable with nickel (Ni)-based superalloys. These materials consist of thermodynamically stable three-phase mixtures of Mo, Mo_3Si, and Mo_5SiB_2, and possess an attractive combination of high melting point (around 2,000 ºC), strong high-temperature oxidation resistance, and excellent corrosion resistance in many environments, making them very interesting for fossil energy applications. However, a fundamental limitation to their utilization is their insufficient fracture toughness and poor ductility at ambient temperature. The project aims to address these limitations through innovative alloying and heat treatment techniques.

Objectives and Technical Approach

The main research objective is to understand the fundamental mechanisms behind embrittlement in Mo and other transitional metal materials due to effects of elemental impurities, and to search for possible means of mitigation. Conventional, theoretical investigations of impurity element embrittlement are usually conducted at or above the atomic level, such as through static energetic analysis and dynamic crack simulations. These approaches lack the required accuracy or efficiency to account for the effects of atomic-level (atomistic) impurities, and often lead to controversial predictions.

PROJECT DURATION

Start Date
08/01/05

End Date
07/31/08

COST

Total Project Value
$278,543

DOE/Non-DOE Share
$200,000 / $78,543

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The present research is focused on ductility enhancement of Mo alloys by adding nano-sized oxide particles to the alloy system. The research approach includes: (1) determination of microscopic mechanisms responsible for the macroscopic ductility enhancement effects through atomistic modeling of the metal-ceramic interface; (2) subsequent computer simulation-aided optimization of composition and nanoparticle size of the dispersion for improved performance; (3) synthesis and characterization of nanoparticle dispersion following the guidance from atomistic computational modeling analyses (e.g., by processing a small sample of Mo alloy for evaluation); and (4) experimental testing of the mechanical properties to determine optimal ductility enhancement.

Accomplishments

Through atomistic modeling and electronic structure analysis using full-potential linearized muffin-tin orbital (FP-LMTO) techniques, research to date has been performed on a number of selected Cr systems containing nitrogen (N) and/or magnesium oxide (MgO) impurities. The emphasis has been on determining the properties of the valence electrons and the characteristics of the chemical bonds they formed. It was found that the brittle/ductile behavior of this transitional metal system is controlled by the relative population of valence charges: bonds formed by *s* valence electrons yield metallic, ductile behavior, whereas bonds formed by *d* valence electrons lead to covalent, brittle behavior. The presence of valence bands from impurities also affects the metal bonding, thereby explaining the detrimental and beneficial effects induced by the inclusion of N impurities and MgO dispersions. These understandings are useful for optimizing ductility enhancement effects on the dispersion materials.

Benefits

This work is expected to lead to a fundamental advancement in understanding of ductility enhancement of Mo, Cr, and other related structural materials. Most current understandings are based on experimental microstructural analyses at the micro-scale level, which cannot adequately explain many of the important mechanical properties including ductility enhancement and its dependence on chemical composition, and nanoparticle size effect, which are determined by electronic and atomic structures at a more fundamental level. Atomistic modeling thus provides indispensable, complimentary, and fundamental knowledge. This knowledge is the starting point for systematic optimization schemes.

Computer simulations also present a comparatively more economical and convenient way to study the important effects caused by variations of material compositions and/or geometries, and to predict the optimal parameters for improved performance, thus reducing the need for time-consuming experimental trial-and-error effort. In addition, the experimental feedback may be used to further improve theoretical modeling capabilities.

As a related benefit, techniques developed in this project can be extended to solve problems in other transitional metal systems. For example, the present work attempts to build a new approach to address the metal-ceramic interface by treating both phases in a consistent framework. Thus the methodology developed should prove useful for other applications such as heterogeneous catalysis, microelectronics, thermal barriers, corrosion protection, and the hydrogen embrittlement in steel.