the ENERGY lab

PROJECT FACTS

Advanced Research

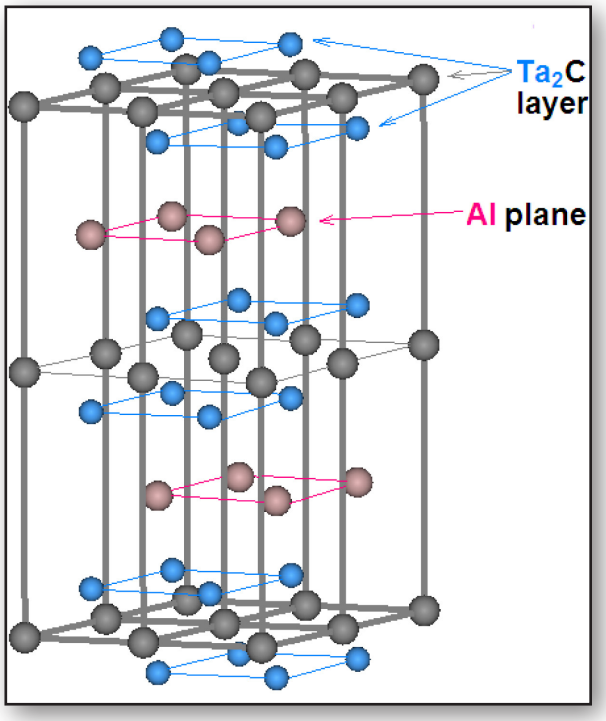
Large Scale Simulations of the Mechanical Properties of Layered Transition Metal Ternary Compounds for FE Power Systems

Background

The U.S. Department of Energy (DOE) promotes the advancement of computational capabilities to develop materials for advanced fossil energy power systems. The DOE's National Energy Technology Laboratory (NETL) Advanced Research (AR) Program is working to enable the next generation of Fossil Energy (FE) power systems. The goal of the AR Materials Program is to conduct research leading to a scientific understanding of high-performance materials capable of service in the hostile environments associated with advanced ultrasupercritical (A-USC) coal-fired power plants.

A-USC plants have the potential to reach higher efficiency, reduce carbon dioxide (CO_2) emissions, and be CO_2 capture ready. In order to develop boiler and steam turbine materials technology for A-USC systems, materials need to be able to withstand and operate at A-USC conditions (760 degrees Celsius [1400 degrees Fahrenheit] and 35 megapascals [5,000 pounds force per square inch]) for at least 20 years.

NETL has teamed with University of Missouri–Kansas City and Tennessee State University to conduct computational studies enabling the search for novel materials or significant improvements in existing materials that can meet requirements of A-USC systems.



Ball and Stick Model of typical MAX Phase (Ta2AlC) Showing the Layered Structure in a 2x2x1 Supercell

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PARTNERS

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PROJECT DURATION

Start Date
08/01/2010

End Date
12/31/2013

COST

Total Project Value
$1,127,346

DOE/Non-DOE Share
$901,877 / $225,469

Project Description

This project focuses on the computational development of a new class of materials called MAX phases, or Mn+1AXn [M = a transition metal, A = aluminum (Al), X = carbon (C) or nitrogen (N)]. The MAX phases are layered transition metal carbides or nitrides with the rare combination of metallic and ceramic properties. Due to their unique structural arrangements and directional bonding (both covalent and ionic) these thermodynamically stable alloys possess some of the most desirable properties such as damage resistance, oxidation resistance, excellent thermal and electric conductivity, machinability, and fully reversible dislocation-based deformation. These properties can be explored in the search for new phases and composites that can meet performance goals set by DOE for applications in A-USC plants.

The project will include the calculation of the electronic structure and mechanical properties of a large number of MAX phase alloys. Based on these results, the search for materials with better thermo-mechanical properties will be performed and the role played by interfaces and internal grain boundaries will be investigated. The project will develop new computational methods and algorithms that can be effectively executed on DOE supercomputers.

The scope of the work is roughly divided into two phases: Phase I will focus on the areas of fundamental mechanical properties, electronic structure and bonding of MAX phase alloys, and execution of the multi-axial tensile/compression simulations. Phase II will focus on mechanical properties in high-temperature, -pressure, and -corrosion environments together with modeling and simulation studies of microstructures and interfaces in MAX phase materials.

Goals/Objectives

The project goal is to predict and understand the mechanical properties of the MAX phase compounds for their potential applications at the extreme conditions of high temperature, high pressure, and highly corrosive environments. The specific objectives are to:

- Systematically study the electronic structure and mechanical properties of a large number of the MAX phase alloys to understand the fundamental physics that lead to these properties.
- Develop new computational algorithms to efficiently and accurately accomplish such calculations and to devise new simulation schemes that will be accurate and predictive for the materials properties at extreme conditions and over prolonged periods of operation.
- Extend the simulations to consider the mechanical properties of microstructure models such as grain boundaries and interphase boundaries both with and without the influence of doped elements; and to use spectroscopic calculations as a means to characterize their composition and structure.
- Explore new material phases within the MAX families and their composite structures that have optimal mechanical and corrosion resistance properties based on information from individual crystals.
- Establish an extensive database of the structure and properties of the modeled MAX systems and provide them to collaborators at DOE laboratories and other institutions so as to accelerate the processing, characterization, and actual application of the new materials.

Benefits

The project will develop new computational methods and algorithms that can be effectively executed on DOE supercomputers. These computational studies can lead the way in the search for novel materials or for significant improvements in existing materials that can meet evolving requirements without incurring costly trial-and-error laboratory tests. At a more fundamental level, detailed computational studies can provide an atomistic level of understanding for the key characteristics that lead to desirable properties. Such studies thereby provide sufficient predictive power to form a viable strategy for the exploration and processing of new materials with a substantial reduction in research and development costs.