TITLE **Ductility Enhancement of Mo Phase by Nano-sized Oxide Dispersions**

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OBJECTIVES

The objective of this research is to understand and to tailor the impurity effects on the ductility properties of molybdenum (Mo) based alloys by the inclusion of nano-sized metal oxide dispersions. Mo based alloys are brittle at room temperature due to oxygen embrittlement. There have been numerous studies concerning improving the ductility of Mo and Cr based alloys at ambient temperature. The purpose of this research is to identify the mechanisms responsible for the impurity embrittling and ductility enhancement based on fundamental electronic structure analysis. Using computational modeling techniques, we aim to develop predictive capabilities to facilitate the designs and optimizations of Mo and other high temperature structural materials for fossil material applications.

ACCOMPLISHMENTS TO DATE

Through first-principles computational modeling and simulations, we investigated the electronic structures of the embrittling species and its effects on hosting metal matrix. The electronic structure provides a detailed description of the properties of the valence electrons that participate in the formation of bonds between atoms in solids. The characteristics of these chemical bonds dictate the mechanical properties of the solids. The purpose is to identify the changes in the microscopic electronic structure due to the presence of impurity elements and to correlate them with the observed changes in mechanical properties. The identified features will be used as criteria to screen other ductility enhancement candidates, for example by varying the composition or size of the metal oxide, for improved performance.

Based on the numerical modeling studies, we also prepared Mo powders mixed with candidate nano-sized oxides, which were then vacuum hot-pressed to make the alloys. The follow-up mechanical properties evaluations were carried out using an in-house developed micro-indentation technique which is suitable for in-situ material mechanical properties and ductility/brittle evaluation of small-size sample alloys.

Theoretical background, experimental verification and relevant test results are presented.

FUTURE WORK

Our future work will include further investigation of ductility enhancement of Cr and Mo related structural materials by suitable oxide dispersions. Using the criteria developed in the mechanism studies and numerical analyses, we will prepared hot-pressed Mo-alloys with optimized nano-sized oxides and experimentally evaluated their enhanced mechanical properties. we will test and optimize the dispersions in terms of composition and size. In addition, the techniques developed in this project will be extended to solve problems in other transition metal systems, such as the hydrogen imbrittlement in steel.

A portable micro-indentation instrument is under development for on-site, in-situ material mechanical property evaluation (Young's modulus, stress/strain curve, hardness, ductile/brittle assessment).

LIST OF PAPER PUBLISHED, U.S. PATENT/PATENT APPLICATION(S), CONFERENCE PRESENTATIONS, AWARDS RECEIVED AS A RESULT OF SUPPORTED RESEARCH, STUDENTS SUPPORTED UNDER THIS GRANT

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