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

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## OBJECTIVES

The objective of this research work is to understand the fundamental mechanisms behind impurity element embrittlement in Mo and other transitional metal systems, and to search for possible mitigations. An example is the ductility enhancement of N embrittled Cr by MgO dispersions, as recently demonstrated by national laboratory scientists Brady, et.al. (*Mater. Sci. & Eng. A358, 243-254, 2003*). 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

Conventional theoretical investigations of impurity embrittlement effects are usually conducted at or above the atomic level, including static energetic analysis and dynamic crack simulations. These approaches lack the required accuracy or efficiency to account for atomistic impurity effects, and often lead to controversial predictions.

Our work is based on electronic structure analysis, which is a level deeper than the conventional approaches. Through atomistic modeling using FP-LMTO techniques, we studied a number of selected Cr systems containing N and/or MgO impurities, with the emphases on the properties of the valence electrons and the characteristics of the chemical bonds they formed. We found that the brittle/ductile behavior of this transition metal system is controlled by the relative population of s and d valence charge: bonds formed by s valence electrons yield metallic, ductile behavior, whereas bonds formed by d valence electrons lead to covalent, brittle behavior. These are in consistent with Rice's criterion. In addition, we found that the presence of 2s bands from impurities such like nitrogen raises Cr's 4s level, resulting in a relatively less occupied s band. In contrast, the presence of 3s valence bands of Mg was found to lower Cr's 4s level, making it more occupied. This explains the detrimental and beneficial effects induced by the inclusion of nitrogen impurities and MgO dispersions as observed in the experiments. These understandings are useful for optimization of the dispersion materials for their improved and robust ductility enhancement effects.

## 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.

## 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

*"Tight-binding study of thermal expansions for Mo3Si",* N.Ma, B.R.Cooper, and B.S.Kang, to appear on J. of Applied Physics, (2006).