Mechanisms of impurity effect and ductility enhancement of Mo and Cr alloys

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Grant Number: DE-FG26-05NT42526
Performance Period: 8/01//2005 to 7/31/2008

OBJECTIVES: The objective of this research is to understand and minimize the impurity effect for room-temperature ductility improvement of Mo- and Cr-based alloys by the inclusion of suitable metal oxide dispersions. Mo- and Cr-based alloys are brittle at room temperature due to oxygen and nitrogen embrittlement, respectively. Past research showed that suitable amount of MgO or $MgAl_2O_4$ dispersion can improve the room temperature tensile ductility of Cr alloys. However, the experimental results were not consistent. MgO dispersions are also potentially useful for ductility enhancement of Mo since the electronic structures and physical properties of the two elements are very similar. The purpose of this research is to identify the mechanisms responsible for the impurity embrittling and to tailor ductility enhancement based on fundamental electronic structure analysis, which will guide the selection of suitable nano-sized metal oxides to be incorporated in the Mo or Cr alloys to achieve the desirable room-temperature ductility. The results will help to formulate systematic strategies in searching for better composed Mo and Cr alloys with optimal mechanical properties.

ACCOMPLISHMENTS TO DATE: On the theoretical analyses, using *ab-initio* FP-LMTO techniques, we investigated the electronic structures of Mo and Cr, with possible embrittling impurities and/or MgO layers. We found that the ductility properties of these systems are correlated to the extent to which the valence electrons near the Fermi level (mostly due to Mo/Cr's d orbitals) are delocalized. The more delocalized these electrons are, the easier the system will be to assume stacking fault configurations. This is consistent with the Rice's criteria on ductile/brittle property. In addition, we found in the brittle systems the density of states (DOS) curve tends to cross the Fermi line at its minimum, while that of a ductile system crosses at its maximum. These observations provide microscopic criteria to predict transition metal's mechanic properties. Finally, we have developed *ab-initio* database for more efficient tight-binding schemes. Such schemes are suitable to study some of the dynamic effects, such as impurity gettering and defects transport, that are pertinent to the ductility enhancement mechanism.

On the experimental verification, we have further developed and refined an indentation technique suitable for in-situ material mechanical property and ductile/brittle evaluation of small size sample alloys. The formation of slip line/shear band is investigated and correlated to the brittle/ductile characterization of the tested alloys.

FUTURE WORK: We will search other metal oxide dispersion candidates for better mechanic performance based on the microscopic criteria we have discovered. In addition, we will study the dynamic effects, including impurity gettering and defects transport, that are pertinent to the ductility enhancement mechanism. These simulations will be carried out using more efficient yet still quantum mechanic based tight-binding schemes. The same schemes will also be employed to conduct larger (nano) scale simulations (10^4-10^5 atoms) to understand the qualitative effects and optimal sizes of nano-sized dispersion particles. Based on the numerical studies, Mo- and Cr-based alloys with suitable nano-sized oxides will be processed with the follow-up experimental mechanical property evaluation to compare and demonstrate improved room-temperature ductility over the existing Mo and Cr alloys.

PUBLICATION:

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CONFERENCE PRESENTATIONS:

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STUDENTS SUPPORTED: Chuanyu Feng and Erin Lin