Quarterly Management Report

WBS Element	Project Title	Contract Number	Contract Start	Contract End
	Integrated Research for Predicting Higher Dimensional Phase Diagrams with Emphasis on Ternary Diagrams of Molybdenum,	4000013127	01/01/02	12/31/04

Performer Name and Address	Principal Investigator(s)
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BUDGET AND COST REPORT

Prior Year Funds [$K]	0
Total Current Year Commitment $K]	0
Projected Current Year Costs [$K]	0

	O	N	D	J	F	M	A	M	J	J	A	S
Planned Costs	0	0	0	0	0	0	0	0	0	0	0	0
Actual Costs	0	0	0	0	0	0	0	0	0	0	0	0
Variance	0	0	0	0	0	0	0	0	0	0	0	0

MILESTONE REPORT

Milestone Designation	Milestone Description	Due Date	Revised Due Date	Completion Date
	Topical Report			07/15/03

TECHNICAL HIGHLIGHTS

In our last quarterly report, we reported our research effort on the modeling analysis of Mo alloys. The aim of this research is to develop a predictive phase diagram ability, including the capability for predicting the ternary system formed by molybdenum, silicon, and boron.

We have modified our tight-binding (TB) parametrization scheme, in which the off-site (hopping) Slater-Koster(SK) parameters were extracted directly from the hamiltonian and overlap matrices computed by full-potential muffin-tin orbital method, based on an orthogonality relationship among the SK coefficients discovered by McMahan et.al. The on-site parameters were augmented to account for both crystal field potential and the ion-ion repulsive potential, in a form that is physically intuitive and free from numerical fitting. The scheme is especially useful in the modeling of intermetallic alloy materials, where the traditional method of obtaining parameters via fitting does not work because of the large number of parameters. We are currently updating this method in an effort to include charge transfer effects for modeling of ionic crystals, such as spinel $MgAl_2O_4$. The structural and physical properties of spinel has gained resurgent interest due to the recent experimental discovery of significant ductility enhancement of Molybdenum based structural materials by spinel dispersions. It is commonly believed that spinel particles will capture or precipitate embrittling impurities such as nitrogen and oxygen ions in the Mo phase, thereby strengthening the structural toughness. However, the exact mechanism is still yet to be found. Through our modeling and simulation of spinel, we proposed the new idea of electrostatic surface potential induced impurity precipitation/segregation along the spinel-Mo boundary to explain the ductility enhancement and decreased oxidation or pest reaction at the Mo grain boundaries. Our TB techniques will be applied to calculate the surface/interface potential, and predict the composition of spinel that renders optimal ductility enhancement.

Our recent microstructural analyses of the tested Mo alloys with spinel particles showed clear experimental evidence of the correlation of MoO_2/ MoO_3 oxides to the detrimental brittle failure of the alloys. We will present our recent research findings at the 18th Fossil Energy Materials Conference (June 2-4, Knoxville, TN). In summary, it is our opinion that lthough $MgAl_2O_4$/MgO oxide-dispersed Mo alloys can improve alloy strength and ductility, further optimization of material processing conditions is needed for better evenly distributed oxide dispersion control and impurity management.

For future research, we propose the following research issues for the Mo alloys development: (i) oxide composition – optimal composition for higher surface electrostatic potential to attract impurity ions, (ii) nano-sized dispersion – optimal nano oxide particle size and more evenly distributed oxide dispersion, (iii) nano-particle synthesis and manufacturing, and (iv) corresponding thermo-mechanical properties and microstructural evaluations.

ISSUES

None

Report Prepared By	**Date**
Bruce S. Kang	05/31/04