Thermodynamic Assessment of the Mo-Re Binary System

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Introduction

One of the approaches to the development of high strength structural materials for high field magnets is the utilization of high modulus alloys that have potential to achieve high strength. Molybdenum-Rhenium (Mo-Re) alloy is one of them. However, the presence of the σ phase in Mo-Re alloys may results in brittleness of the alloys. To understand the conditions for formation of σ phase and the other brittle phases, we evaluated the phase diagrams. Despite the broad applications of the Mo-Re alloys, part of the phase diagram remains unclear. We reviewed the previous experimental data, and calculated the thermodynamic parameters and the phase diagram of the Mo-Re system. Special attention has been given to the thermodynamic description of the brittle σ and χ phases.

Results and Discussion

The liquid, bcc and hcp phases were treated as disordered substitutional solutions of Mo and Re. The σ phase belongs to the space group of D_{4h}^{14}-$P4_2/mnm$, as shown in Fig. 1a and b. The tetragonal unit cell contains 30 atoms [15] and they occupy five crystallographically different sites, which are designated as A, B, C, D and E with 2, 4, 8, 8, and 8 atoms in each of the sites. The coordination numbers (CN) for sites A, B, C, D and E is 12, 15, 14, 12 and 14 respectively. Thus the σ phase crystallographical structure can be simply written as $(A)^{12}{}_2(B)^{15}{}_4(C)^{14}{}_8(D)^{12}{}_8(E)^{14}{}_8$. We simplified the structure. The models of the σ phase are used in the present study are $(Re)_8(Mo)_4(Mo,Re)_{18}$ $(Re)_{10}(Mo)_4(Mo,Re)_{16}$. χ phase belongs to the space group of T_d^3—I43m. It is a bcc phase with 58 atoms per unit cell. Of the 58 atoms, 10 have the coordination number of CN16, 24 have the coordination number of CN12, and the remaining 24 have CN 13. The present Mo-Re system describes the χ phase as three sublattices: $(Re)_{24}(Mo)_{10}(Re,Mo)_{24}$.
The model parameters were assessed and calculated. We calculated the parameters by minimizing the error sum with weighted experimental data. The weight for a variety of experimental data was chosen by trial and error and adjusted based on the data uncertainties given in the original publications. The Gibbs energies of all the phases in Re-Mo obtained in the present work are shown in reference 1. The Mo-Re binary phase diagram calculated by our model is presented in Fig.1.
Some of the important results of our thermal calculation are:

1. The solubility of Re in (Mo) is significantly higher than Mo in (Re) and the extrapolated solubility of Mo in (Re) is smaller than $5x10^{-4}$ mole at room temperature;
2. The melting points of (Re) and (Mo) are determined from our calculations;
3. χ phase is stable above 1000 K and the composition range for χ phase is smaller than experimental data;
4. σ phase decomposes at 1375 K.

Acknowledgements

This project is partially supported by an IHRP fund.

References

[1] Mao, PL, Han, K and Xin, Y, Journal of Alloys and Coumpounds, Accepted for publications

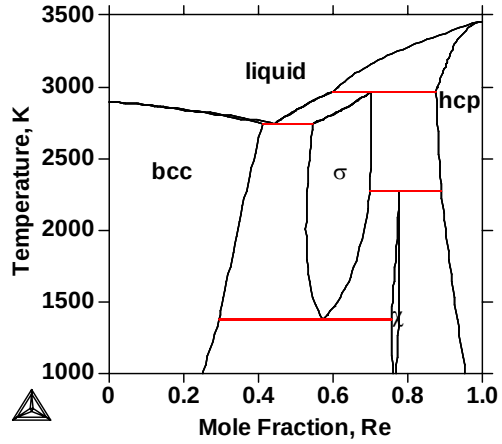

Fig.1 Calculated Mo-Re system equilibrium phase diagram