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Phase formation, phase equilibria and phase transformation of the Ag-Cu-Se-Te quaternary system

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Introduction

The phase diagram is indispensable to understanding the phase formation or transformation, designing new alloys for advanced application, and optimizing the material processing. This study is to determine the phase equilibria of the Ag-Cu-Te-Se quaternary system. The experimental determination and thermodynamic modeling of CALculation of PHAse Diagram CALPHAD-method are used to study the system. The phase diagram of Cu-Te and Ag-Se binary systems are calculated. The phase diagram of Cu-Se-Te and Ag-Cu-Se ternary systems will be presented.

Results

Calculated Cu-Te and Ag-Se binary phase diagrams

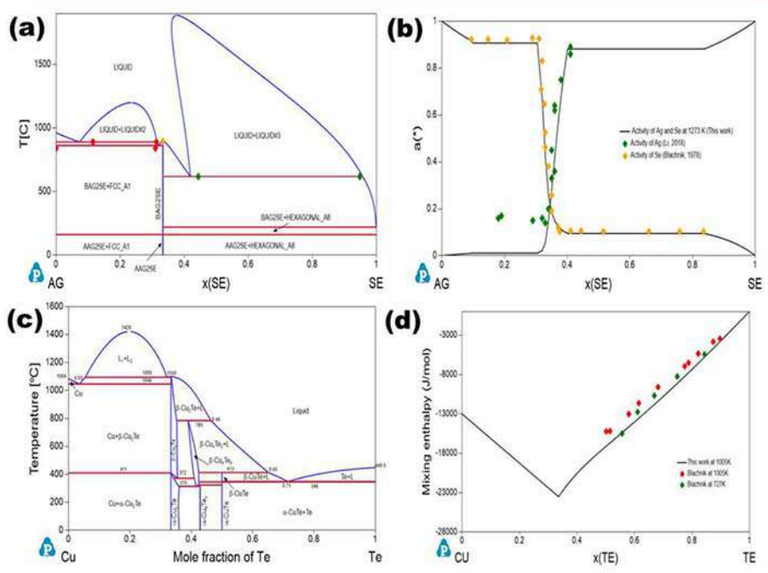

Fig.1: (a) Phase diagram of Ag-Se, (b) Activity of Ag and Se at 1273K, (c) Phase diagram of Cu-Te, (d) Enthalpy of mixing of liquid at 1005K.

New thermodynamics description parameters are obtained to model the Cu-Te and Ag-Se binary systems. The optimization was carried out based on the minimization of the Gibbs free energy of the system by using Pandat Software. As shown in Figure 1(a-d), the phase diagrams and thermodynamic properties results show good agreement with the literature.

Calculated Cu-Se-Te ternary phase diagram

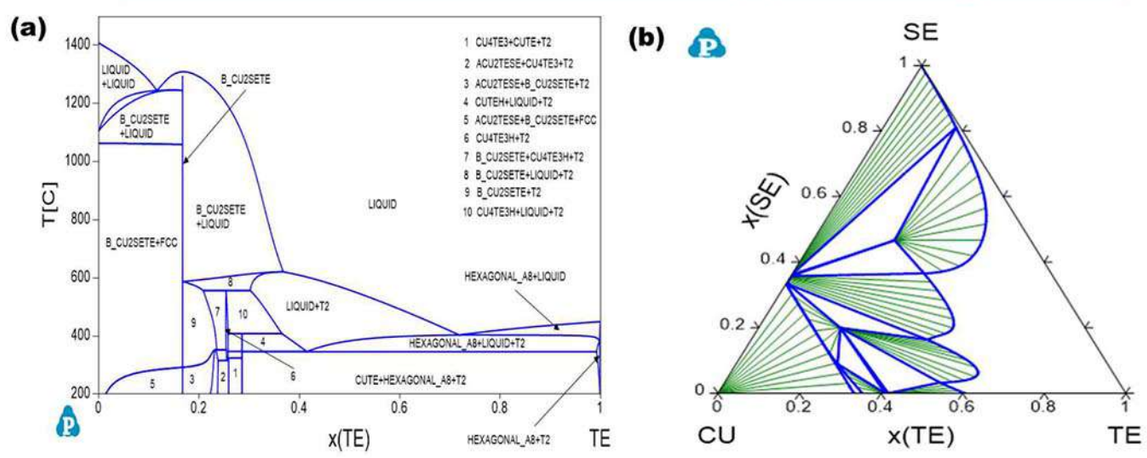

Fig.2: Phase diagram of Cu-Se-Te ternary system: (a) The isopleth section of Cu_2Se-Te and (b) the isothermal section 500°C

Based on the three constituent binary phase diagram of Cu-Te, Cu-Se, and Se-Te systems and from the information of ternary experimental results, the phase diagram of the Cu-Se-Te ternary system is calculated. The isopleth and isothermal sections of the system are shown in Figures 2a and 2b, respectively.

Ag-Cu-Se isothermal section at 500°C

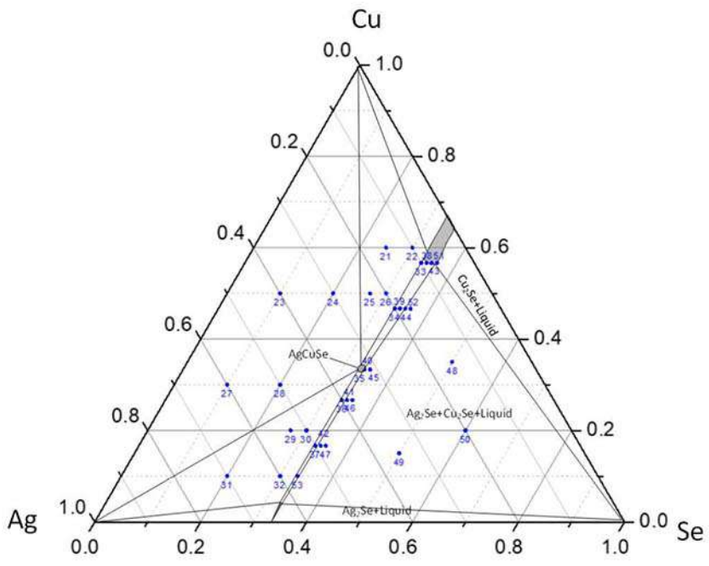

Fig.3: The determined isothermal section of Ag-Cu-Se ternary system at 500°C

Three constituent binary phase diagrams of Ag-Cu, Ag-Se, and Cu-Se are selected to give an equilibrium phase information at each side. At 500 °C, they are (Ag,Cu), Cu_2Se, and Ag_2Se phases on each side of Ag-Cu, Ag-Se, and Cu-Se, respectively. The solution phases are Ag, Cu, and liquid (Se). The isothermal section of Ag-Cu-Se system was determined by analyzing the equilibrated alloys at 500°C. As shown in Fig. 3, there are four tie-triangles in the isothermal section at 500°C. The ternary compound of AgCuSe was found.

Ag-Cu-Se isothermal section at 300°C

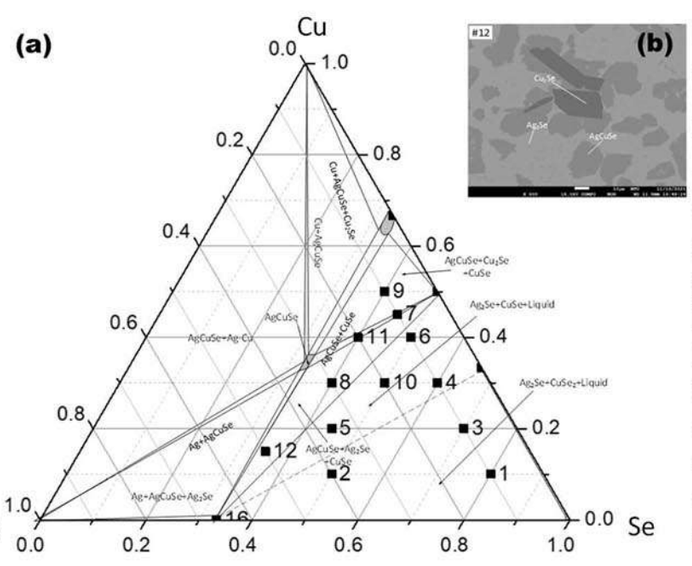

Fig.4: (a) The determined isothermal section of Ag-Cu-Se ternary system at 300°C and (b) BEI micrograph of alloy #12

Following a similar analytical determination, the equilibrium phases at 300°C were determined. The equilibrium phases on the Cu-Se side are Cu_2Se, CuSe, and $CuSe_2$. As shown in Fig. 4(a), there are seven tie-triangles in the isothermal section at 300°C. The ternary compound of AgCuSe was found. The BEI micrograph of alloy #12 is shown in Figure 4b. It shows three phases in equilibrium: Ag_2Se, CuSe, and AgCuSe.

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Research experience

2016-2018: Master degree research project on Bi-In-Se system: (*Calphad Journal*. 68 (2020): 101744) and (*J. Alloys Compd* 779 (2019): 347-359). ChE, NTHU.
2018-2019: Research assistant in Institute of Physics in Academia Sinica: (Adv Sci (2022): 2201353)
2019-now: PhD Candidate in Department of ChE, NTHU. Taiwan

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