927℃ Nb-Si-Ge 與 600℃ Cu-Si-Ge 兩三元平衡相圖之研究

[**摘要**]

In this thesis , the semiconductor-rich region of the Nb-Si-Ge ternary isotherm at 927℃ and the Cu-Si-Ge ternary isotherm at 600℃ were determined by using X-ray diffraction、electron-probe microanalysis and metallography. The main objective is to provide the necessary thermodynamic information for designing contact materials for applications in SiGe or Si devices.

In the second part of this thesis, the diffusion behaviors of Cu-Si-Ge system were preliminarily studied. The objective is to provide the kinetic information for understanding the reaction between Cu and SiGe.

It was confirmed that at 927℃ NbSi2 and NbGe2 form a continuous solid solution Nb(Si1-xGex) with the C40 crystal structure. It was also shown that, other than Nb(Si1-xGex) and Si1-yGey , there is no known binary or ternary phase within the Si-Ge- NbGe2- NbSi2 trapezoid. The lattice parameters of Nb(Si1-xGex) were determined. The tie-lines for the Nb(Si1-xGex)- Si1-yGey two phase region tilt slightly toward the NbSi2 and Ge corners presumably because the enthalpy of formation for NbSi2 is more negative than that of NbGe2. The tie-lines also show that the NbSi2 and NbGe2 are not stable when they are in contact with SiGe solid solution alone.

In the Cu-Si-Ge ternary isotherm study at 600℃ study, we confirmed that Cu7Si and Cu5Ge formed a continuous solid solution with the A3 crystal structure ,but Cu3Si and Cu3Ge didn’t. We found that the crystal structure information of e1-Cu3Ge in the ”Pearson’s Handbook of Crystallographic Data for Intermetallic Phases” could have some errors. The diffraction pattern of ε-Cu3Ge and ε1-Cu3Ge could be the same. Otherwise the stably existing temperature of ε-Cu3Ge and ε1-Cu3Ge in the Cu-Ge binary phase diagram would have wrongs. The Si would slightly dissolve into Cu3Ge to form the Cu3(Si1-xGex) with low electrical resistivity close to Cu3Ge and the Cu3(Si1-xGex) would be stable on the SiGe substrate. Therefore, we can use this property of Cu3(Si1-xGex) to design the stable contact material on the SiGe substrate.

In the second part of this thesis, Cu/Ge binary diffusion couple experiment at 600℃ was performed. The growing rate of the Cu3Ge phase is greater than that of the Cu5Ge phase. The one and only crystal structure of the Cu3Ge phase was detected. We assumed that the stably existing temperature of the Cu3Ge phase with different crystal structures in the Cu-Ge binary phase diagram had some errors, or the variation in interdiffusion coefficients between the two different crystal structures of the Cu3Ge phase was large. We found that no detectable reaction in the Cu/Si binary diffusion couple occurred at 600℃. The main objective is to provide the necessary thermodynamic information for NbSi2 and Cu3Ge when they contact with SiGe or Si substrate. The information would be a great benefit to the development of metallization for the new contact materials in the microelectronic industrial.