Experimental Investigation of the Si-Ge-Ti Ternary Phase Diagram and Diffusion Behaviors

ABSTRACT

In this thesis, the Si-Ge-Ti ternary isotherm at 900 ^{o}C was determined by using metallography, x-ray diffraction, and electron microprobe. The main objective is to provide the necessary thermodynamic information for designing contact materials in SiGe devices. In the second part of this thesis, the diffusion behaviors of Si-Ge-Ti system were studied. The objective is to provide the kinetic information for understanding the reactions between Ti and SiGe.

In this study, it was confirmed that at 900 ^{o}C $TiSi_2$ and $TiGe_2$ form a continuous solid solution with the C54 crystal structure. It was also shown that, other than $Ti(Si_{1-y}Ge_y)_2$ and $Si_{1-x}Ge_x$, there is not any binary or ternary phase within the Si-Ge-$TiGe_2$-$TiSi_2$ trapezoid. Between the $Ti(Si_{1-y}Ge_y)_2$ and $Si_{1-x}Ge_x$ single-phase field is the $Ti(Si_{1-y}Ge_y)_2$-$Si_{1-x}Ge_x$ two-phase region. The tie-lines for the $Ti(Si_{1-y}Ge_y)_2$-$Si_{1-x}Ge_x$ two-phase region were determined. The tie-lines tilt slightly toward the $TiSi_2$ and Ge corners presumably because the enthalpy of formation for $TiSi_2$ is slightly more negative than that of $TiGe_2$. In other words, at equilibrium the silicon to germanium atom ratio is larger in the $Ti(Si_{1-y}Ge_y)_2$ phase than in the $Si_{1-x}Ge_x$ phase ($x>y$). The isotherm determined here was then used to explain the complicated phenomena observed during the reaction between Ti and $Si_{1-x}Ge_x$. A strategy of forming stable contact to SiGe device was devised based on the thermodynamic information obtained in this study.

It was also confirmed that at 900 ^{o}C and 1100 ^{o}C Ti_5Si_3 and Ti_5Ge_3 form a continuous solid solution with the $D8_8$ crystal structure. The lattice parameters of $Ti_5(Si_{1-w}Ge_w)_3$ were determined. The homogeneity ranges of $Ti_3(Si_{1-v}Ge_v)$, $Ti(Si_{1-q}Ge_q)$, $Ti_5(Si_{1-p}Ge_p)_4$, and $Ti_6(Si_{1-r}Ge_r)_5$ solid solution were also determined.

In the second part of this thesis, Ti/Ge binary diffusion couple experiment at 800 ^{o}C was performed. Two of the three thermodynamically stable phases, Ti_6Ge_5 and $TiGe_2$, were identified. However, Ti_5Ge_3, which is

also stable at 800 ^{o}C, was not detected. Reasons for Ti_5Ge_3 to be missing were discussed.