Experimental investigation of the Si-Ge-Co ternary phase diagram and diffusion reactions

ABSTRACT

In this thesis, the Si-Ge-Ni ternary isotherm at 750 ^{o}C was determined by using metallography, electron microanalysis, and x-ray diffraction. The main objective is to provide the necessary thermodynamic information for designing contact materials for the SiGe devices. In the second part of this thesis, the diffusion behavior of Si-Ge-Ni system was preliminarily studied. The objective is to provide the kinetic information for understanding the reactions between Ni and SiGe.

In the semiconductor-rich region, it was confirmed that at 750 ^{o}C NiSi and NiGe form a continuous solid solution Ni($Si_{1-y}Ge_y$) with the B31 crystal structure. The lattice parameters of Ni($Si_{1-y}Ge_y$) were determined. Because the three phase region $Si_{1-x}Ge_x$-Ni($Si_{1-y}Ge_y$)-Ni($Si_{1-w}Ge_w$)$_2$ is very narrow, the region between the Ni($Si_{1-y}Ge_y$) and $Si_{1-x}Ge_x$ single phase fields is almost completely occupied by the Ni($Si_{1-y}Ge_y$)-$Si_{1-x}Ge_x$ two phase field. The tie-lines for the Ni($Si_{1-y}Ge_y$)-$Si_{1-x}Ge_x$ two phase region were determined. The tie-lines tilt slightly toward the NiSi and Ge corners presumably because the enthalpy of formation for NiSi is more negative than that of NiGe. In other words, at equilibrium the silicon to germanium atom ratio is larger in the Ni($Si_{1-y}Ge_y$) 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 Ni and $Si_{1-x}Ge_x$. A strategy for forming stable contact to SiGe device was devised based on the thermodynamic information obtained in this study.

The Nickel-rich region was also determined in this study. The complete Si-Ge-Ni ternary isotherm was therefore established.

In the second part of this thesis, the diffusion path of $NiSi_2$ and Ge at

950 ^{o}C was determined. Form this study, the composition of $Si_{1-x}Ge_x$ that can be in equilibrium with $NiSi_2$ at 950 ^{o}C was determined to be x=0.08.