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

ABSTRACT

In this thesis, the Si-Ge-Co ternary isotherm at 800°C was re-determined by 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 devices. In the second part of this thesis, the diffusion behaviors of Si-Ge-Co system were studied. The objective is to provide the kinetic information for understanding the reaction between Co and SiGe.

It was shown that despite rather long annealing times, the silicon-germanium phase did not come fully into homogeneity in composition. It was caused by severe segregation and slow diffusion in silicon-germanium. It was also shown that Co_5Ge_7 is not stable at 800 °C and it decomposes at 797 °C. The composition of $Si_{1-x}Ge_x$ that can be in equilibrium with $CoSi_2$ was determined to be x=0.78. The tie-lines in the two-phase equilibrium between $Si_{1-x}Ge_x$ and $Co(Si_{1-y}Ge_y)$ were also determined. The isotherm determined here was then used to explain the complicated phenomena observed during the reaction between Co and $Si_{1-x}Ge_x$. A strategy of forming stable contact to SiGe device was devised based on the thermodynamic information obtained in the study.

The cobalt-rich region of the Si-Ge-Co ternary phase diagram was also established. These results together with those mentioned above fully describe the Si-Ge-Co ternary phase equilibria at 800°C.

In the second part of this thesis, Co/Ge binary diffusion couple experiment at 800° C was performed. Two of the three thermodynamically stable phases, Co₃Ge₂ and CoGe,

were identified. However, $CoGe_2$, which is also stable at 800 °C , was not detected. Reason for $CoGe_2$ to be missing was probably the large difference in interdiffusion coefficients. The Co/CoGe binary diffusion couple experiment at 800°C was also performed. The reaction was very rapid. It was found that voids near the Co/Co₃Ge₂ interface caused by thermal stress between Co and Co₃Ge₂.