Kinetics of Phase Formation in Ni-Co-Si Ternary system using Bilayer and Alloyed thin films

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From 5G to automotive tech, next-generation microelectronic circuits hinge on high-performance nanometric MOS transistors. Central to these devices are silicides of Co and Ni, which are essential for creating low-resistance contacts that ensure optimal functionality and elevate semiconductor performance [1]. These contacts are obtained by solid state reaction between a metal film and the Si substrate. This study explores the phase formation kinetics in thin films of Ni and Co silicides, with a focus on the ternary Ni-Co-Si system. By integrating in situ experimental techniques and computational simulations, this work explores the relationship between phase formation, metal distribution, and the Ni-Co-Si phase diagram under thermal annealing conditions.

Bilayer thin films with varying Ni and Co thicknesses and as well as the corresponding alloys films (figure 1), were thermally annealed under different conditions to study the sequences of phases and kinetics of phase formation. After cleaning the silicon substrate, Co and Ni bilayer and alloys films were deposited using magnetron sputtering using Co and Ni targets. In situ X-ray diffraction (XRD) was employed to observe real-time phase evolution during step annealing with increasing temperatures, complemented by isothermal XRD annealing for detailed phase transition analysis. Resistance measurements were also conducted to observe the changes in electrical properties as the silicides formed. To understand the atomic-scale distribution of nickel and cobalt during phase formation, atom probe tomography (APT) was utilized. APT provided high-resolution, three-dimensional maps of the elemental distribution.

The results (figure 2) show that nickel significantly influences the formation temperatures of CoSi and MSi_2 phases, accelerating their growth. The diffusion of nickel occurs faster than cobalt, consistent with theoretical expectations. In bilayer films, the simultaneous growth of NiSi and CoSi phases was observed, notably when the nickel concentration exceeded 25%, which agrees with phase diagram predictions. Additionally, the study highlights the role of film composition and thickness in tuning phase transitions and silicide stability. The formation temperature of the M_2Si phase varies based on the initial layer in contact with silicon (figure 3). The M2Si formation temperature is ~280°C when nickel contacts silicon but increases with cobalt thickness when the Co layer is in contact with Si, confirming Co layer as a diffusion barrier. Higher cobalt concentrations also raise the temperature for complete M2Si consumption. These results can be described using the ternary phase diagram (Figure 4). This research gives valuable insights into silicide formation mechanisms and their impact on device performance, contributing a new path for optimizing contact materials in advanced microelectronic circuits.

References

1. D. Mangelinck, The Growth of Silicides and Germanides, Handbook of Solid-State Diffusion, 2017.
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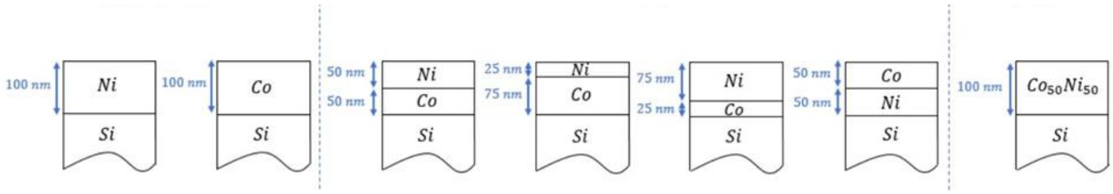

Figure1. Schematic representation of samples analyzed

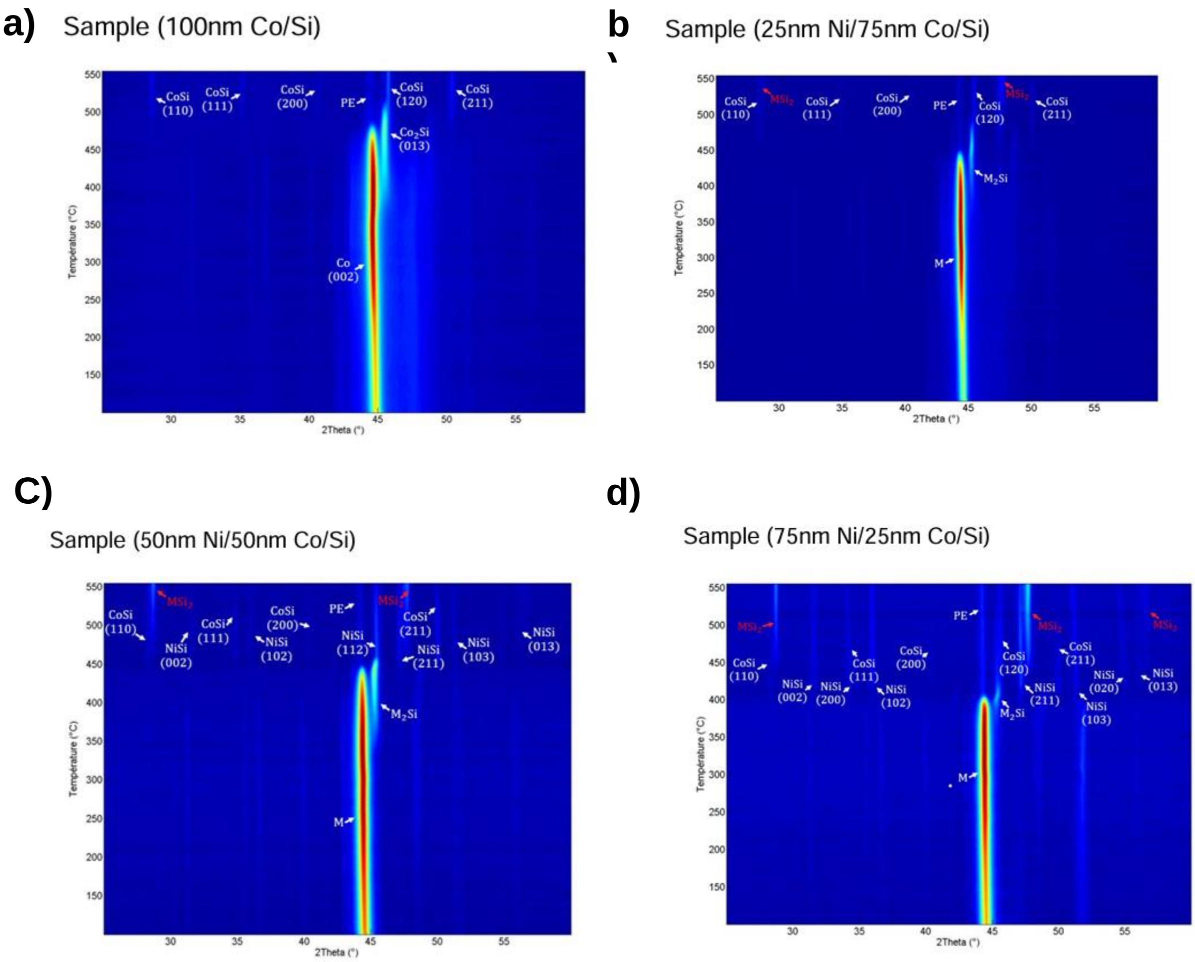

Figure 2. In situ XRD patterns for the bilayer samples

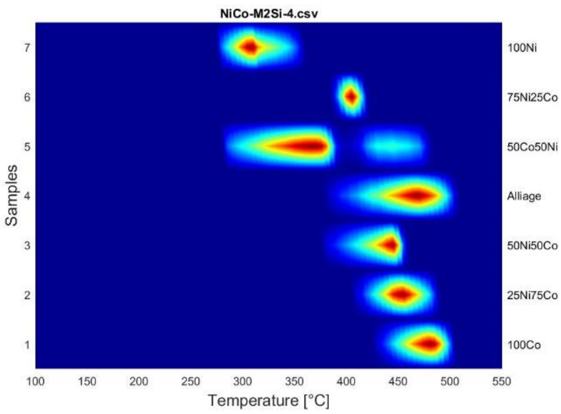

Figure 3. Comparative kinetics of the M2Si phase in the different samples

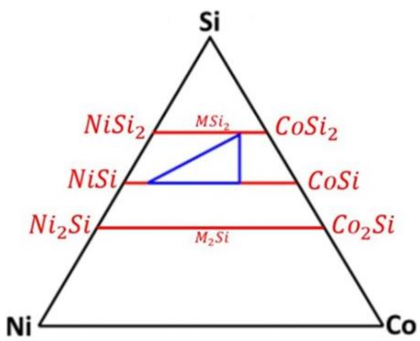

Figure 4. calculated Co-Ni-Si ternary phase diagram at 400[0]C for thin film reaction. The equilibrium between CoSi, NiSi, and MSi_2 is drawn in blue