Reactive diffusion in Ni-Co-Si Ternary system using Bilayer and Alloyed thin films

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From 5G to automotive technologies, next-generation microelectronic circuits hinge on high-performance nanometric MOS transistors. Metal silicides are essential in CMOS technology as contacts for source, drain, and gate regions, reducing resistivity and enhancing device efficiency. These contacts are obtained by solid-state reaction between a metal film and the Si substrate [1]. $TiSi_2$ and $CoSi_2$ were widely used contacts but exhibited resistivity issues at submicron dimensions. In contrast, NiSi, although having a line-width-independent formation, suffers from poor thermal stability due to its transformation into $NiSi_2$ above 700 °C or to agglomeration at temperatures as low as 500°C for very thin films. To overcome these drawbacks, alloyed silicides are being investigated to improve the formation and stability of the silicides [2,3]. This study focuses on the phase formation kinetics in Co silicide alloys for the Ni-Co-Si systems. The effect of Ni on the phase evolution and the kinetics of silicide formation by reactive diffusion is investigated using in situ techniques and simulations.

Bilayer thin films with varying Ni and Co thicknesses, as well as the corresponding alloy thin 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 with HF, Co and Ni bilayer and alloy films with varying Ni compositions (25%, 50%, and 75%) were deposited using magnetron sputtering from Co and Ni targets. In situ X-ray diffraction (XRD) was employed to observe the real-time phase evolution during step annealing at increasing temperatures, complemented by isothermal XRD annealing for detailed analysis of phase transitions and kinetics. In situ sheet resistance measurements were also conducted using a four-probe method to observe the changes in phase formation as well as the electrical properties of the silicides as they formed.

The main phases observed are the metal-rich phase $(Co1\text{-}xNix)_2Si$, the two monosilicides based on CoSi and NiSi, and the silicon-rich phase $(Co_{1-x}Ni_x)Si_2$. (Figure 2). The XRD results indicate that nickel significantly accelerates the formation of M_2Si, MSi, and MSi_2 silicide phases (M indicates the $Co_{1-x}Ni_x$ mixture of Ni and Co). Growth kinetics of the phases are increased by the composition of Ni, as Ni is the fastest diffusing species. The formation temperature of the M_2Si, MSi, and MSi_2 phases reduces as the concentration of Ni increases (Fig. 3). In bilayer films, the simultaneous formation of NiSi and CoSi phases was observed, especially when the Ni concentration exceeded 25%. However, there is no formation of NiSi observed for 25% Ni in the sample, which is due to the solubility limit of Ni in the metal sublattice. These results can be described using the ternary phase diagram (Fig. 4). The simulations using a reaction/diffusion-controlled growth model of the in situ XRD measurements allowed us to determine the growth kinetic parameter of the M_2Si phase. For increasing Ni concentration, the activation energy for diffusion shows a decreasing trend, indicating a reduction in the kinetic barrier for diffusion. In situ sheet resistance measurements show that increasing the Ni concentration shifts the transition from high to low sheet resistance to a lower formation temperature of the phases (Fig. 5). This indicates that the Nickel in the film influences the phase formation kinetics of the phases and the resistivity changes accordingly. This research gives valuable insights into silicide formation mechanisms and their impact on device performance, contributing to a new path for optimizing contact materials in advanced microelectronic circuits.

References

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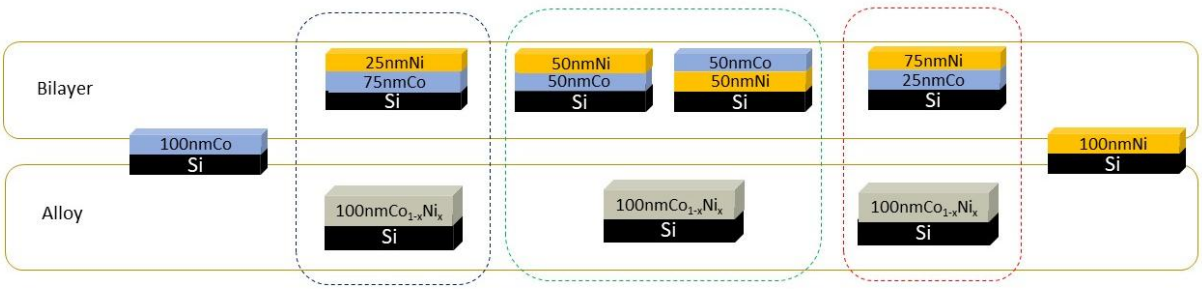

Figure1. Schematic representation of samples analyzed

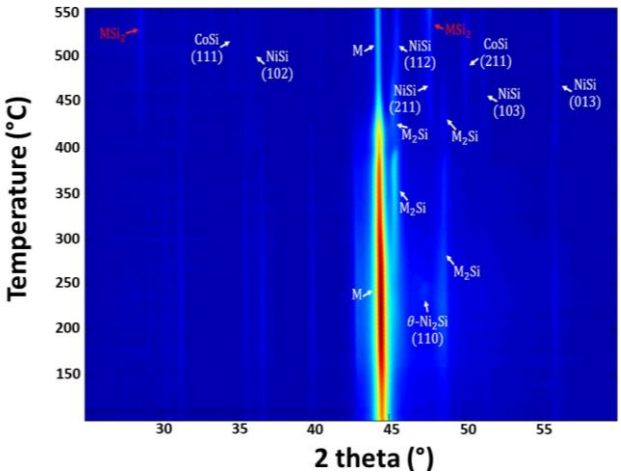

Figure 2. In situ XRD patterns for the bilayer sample 50nmNi/50nmCo/Si

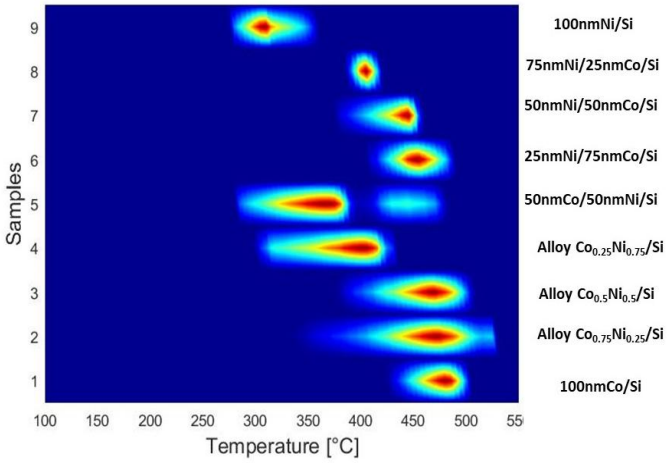

Figure 3. Comparative kinetics of the M_2Si phase in the different samples

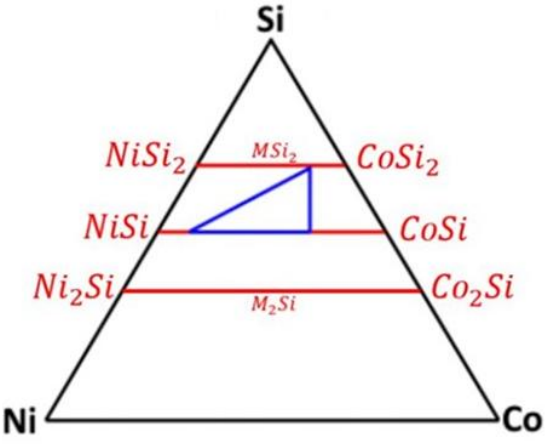

Figure 4. Calculated Co-Ni-Si ternary phase diagram at 400°C for thin film reaction. The equilibrium between CoSi, NiSi, and MSi_2 is drawn in blue

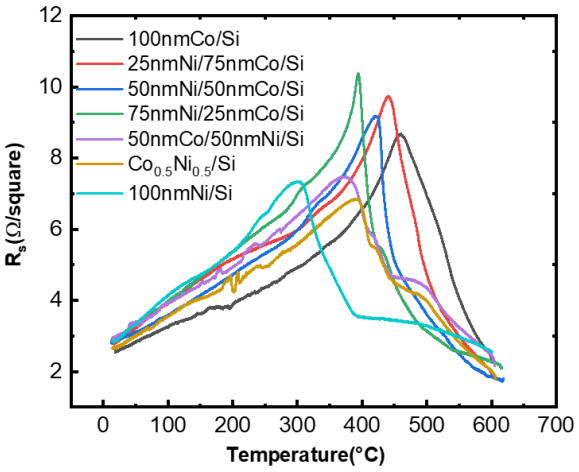

Figure 5. In situ Sheet resistance as a function of Temperature of the Ni-Co-Si samples