Formation of ternary nickel dislicide films with modified lattice parameters: influence of Al and Ga

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Silicides are chemical compounds of silicon with different metals. Favourable electrical properties of metallic silicides as well as their excellent compatibility with Si have made them attractive for the use in microelectronics as ohmic contacts, Schottky barrier contacts, local interconnects and gate electrodes.

Commonly, epitaxial silicide films exhibit undesirable strain. Richter et al. showed that substitution of Si by Al or Ga results in a change of the lattice parameter of bulk $NiSi_2$ [1]. The zero lattice match to silicon is reached for $NiSi_{1.74}Al_{0.26}$ and $NiSi_{1.83}Ga_{0.17}$ at room temperature. This reveals a possibility to grow defect-free lattice matched nickel disilicide films, which is challenging for both technological and fundamental research. Among all transition metal silicides cubic nickel dislicide $NiSi_2$ shows the smallest lattice mismatch to Si (about -0.5 %). Despite that the growth of closed, unstrained and uniformly oriented $NiSi_2$ layers on Si(001) is a difficult task. Commonly, pure $NiSi_2$ forms pyramidal islands on Si(001) with two different orientations (A- and B-type). In our study thin Ni/Al and Ni/Ga layers of different atomic ratios were codeposited onto Si(001) at room temperature followed by subsequent annealing. The influence of Al resp. Ga content as well as the annealing temperature on morphology and composition of ternary $NiSi_{2-x}Al_x$ and $NiSi_{2-x}Ga_x$ layers was investigated by transmission electron microscopy comprising conventional TEM, EDXS and STEM. Additionally, quantitative HRTEM will be used for lattice strain analysis to estimate the change of the lattice mismatch as a function of Al resp. Ga content.

It has been shown that the addition of Al leads to a change in the layer morphology [2]. Separated $NiSi_2$ islands with the A- and B-type orientations are observed after annealing of a 20 nm thick Ni film on Si(001) at temperatures above 800 °C (Fig. 1). The annealing of Ni/Al films on Si(001) leads to the formation of closed $NiSi_{2-x}Al_x$ layers of A-type (Fig. 1). The layer roughness strongly depends on the Al content. Almost smooth layers are obtained for Al content z ranging from 0.2 to 0.3. Furthermore, introduction of Al into the Ni-Si thin film system leads to a decrease of the disilicide formation temperature from 750 °C for a pure Ni film on Si down to at least 500°C for the Ni/Al thin film system. Isolated $NiSi_2$ crystallites of about 10 nm in size were observed after 500 °C annealing at the NiSi/Si interface already at an Al content z of 0.06 (Fig. 2a). An increase of Al content up to z = 0.2…0.3 leads to formation of a closed $NiSi_{2-x}Al_x$ layer appearing at the interface between a cubic polycrystalline $NiSi_{0.5}Al_{0.5}$ film and the Si substrate (Fig. 2b, c).

Similarly to the Ni/Al thin film system on Si an addition of Ga leads to a decrease of the disilicide formation temperature. For a Ga content z = 0.22…0.28 epitaxial A-type oriented grains of pure $NiSi_2$ were observed already after annealing at 450 °C (Fig. 3a). These grains are formed at the interface between a top-layer containing Ni, Ga as well as Si and the

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Si substrate. According to EDXS analysis the composition of the top-layer is not uniform suggesting the simultaneous presence of different Ga-Ni-Si compounds.

An annealing above 900 °C leads to formation of closed epitaxial A-type $NiSi_{2-x}Ga_x$ layers (Fig. 3b) with a homogeneous Ga distribution across the layer. The interfacial roughness varies locally up to 30 nm due to the presence of the $NiSi_{2-x}Ga_x\{111\}$ facets. Thus, further experiments are required to optimize the layer roughness.

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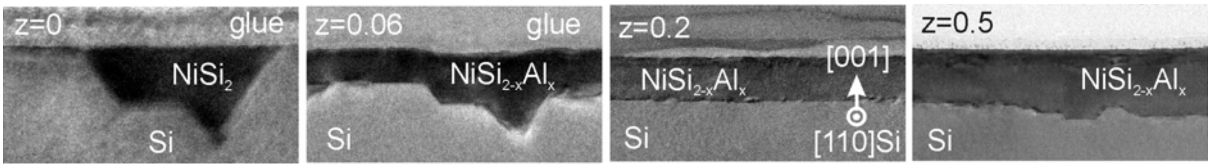

Figure 1. Cross-sectional TEM images of Ni/Al layers codeposited onto Si(001) using different Ni/Al = 1/z ratios and subsequently annealed at 900 °C.

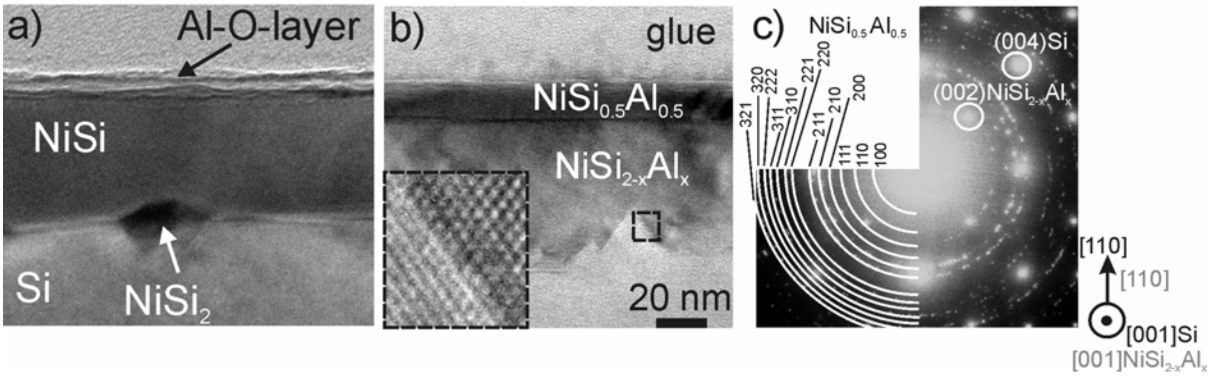

Figure 2. Cross-sectional TEM images of Ni/Al layers codeposited onto Si(001) using different Ni/Al = 1/z ratios a) z = 0.06 and b) z = 0.2 after annealing at 500 °C. The inset in b) shows a high-resolution image of A-type oriented disilicide $NiSi_{2-x}Al_x$. c) Plan-view diffraction pattern proving the simultaneous presence of epitaxial $NiSi_{2-x}Al_x$ and polycrystalline $NiSi_{0.5}Al_{0.5}$ for z = 0.2 (see cross-section in b)).

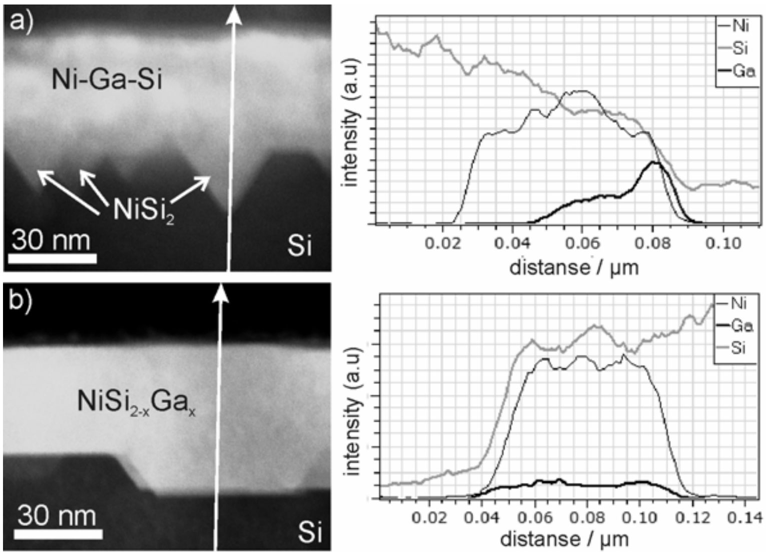

Figure 3. Cross-sectional HAADF STEM images and the corresponding EDXS line scans of sample with a Ga content z of 0.28 after annealing at a) 450 °C and b) 900 °C. Pyramidal grains of pure $NiSi_2$ are visible in a) at the interface between the top layer containing an inhomogeneous mixture of Ni, Ga and Si and the Si substrate. After a 900 °C annealing Ga is homogeneously distributed across the disilicide layer.