Reduced compositional fluctuations in epitaxial NiAl layers

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As interconnect dimensions scale down, it is well established that the resistivity of Cu increases significantly due to enhanced electron scattering at surfaces and grain boundaries. These effects, coupled with the challenges associated with metallizing sub-10 nm interconnect lines and the difficulty of scaling diffusion barriers in advanced technology nodes, present substantial limitations for future copper-based metallization schemes. Consequently, there is growing interest in exploring alternative materials and metallization strategies for next-generation interconnects. Extensive investigations have been conducted in recent years, both on elemental metals and binary intermetallic compounds, to identify suitable candidates for this application [1, 2].

NiAl has emerged as a promising binary intermetallic candidate due to its low bulk resistivity of 9 μΩcm, negligible diffusion into SiO_2, and strong adhesion with common dielectrics. These characteristics make NiAl a potential option for barrier- and liner-free interconnects [3]. However, a critical limitation of NiAl is its susceptibility to compositional fluctuations, which are detrimental to thin film and interconnect resistivities, severely hindering its practical implementation as a next-generation interconnect material [4]. Moreover, the length scale of these fluctuations is on the order of the targeted interconnect line width, significantly affecting etch and clean processes. Addressing this issue necessitates advanced characterization techniques to elucidate the underlying mechanisms driving these inhomogeneities. It has been demonstrated that the growth of epitaxial NiAl on (100) Ge substrate reduces resistivity by optimizing the grain microstructure [5].

In this work, we study potential compositional inhomogeneities in epitaxial NiAl thin films. Epitaxial NiAl (100) layers were deposited by co-sputtering at 420°C onto 500 nm thick strain-relaxed chemical vapor deposition (CVD) Ge grown on 300 mm Si (100) wafers. The microstructure and compositional uniformity of the films were characterized using advanced techniques including atom probe tomography (APT), which enabled the assessment of the spatial distribution of the atomic composition. The spectrum obtained from a 5-nm-thick cylindrical region of interest (ROI) (Figure 1) indicates a stoichiometric composition within the sample. A ~2% Ge content observed within the ROI arises from interdiffusion at the NiAl/Ge interface.

Structural analysis, including X-ray diffraction (XRD) θ-2θ scans and reciprocal space mapping (RSM), confirms the high-quality epitaxial growth of NiAl. The out-of-plane orientation was determined to be NiAl (100) ‖ Ge (100) ‖ Si (100), with an in-plane relationship of NiAl (010) ‖ Ge (010) ‖ Si (010). RSM data for NiAl (202) (Figure 2) reveals lattice constants corresponding to less than 1% deviation from the bulk NiAl lattice parameter (a_0=2.86 Å), indicating a relaxed epitaxial structure.

Figure 3 presents the concentration profile along the length of the sub-cylinder, revealing an uniform distribution of Ni and Al. Furthermore, a compositional histogram (Figure 4), calculated using a 2nm radius around each reconstructed atom, demonstrates significantly reduced fluctuations compared to the uneven distribution observed in polycrystalline NiAl on SiO_2. The comparison with a random comparator (shuffled dataset) yields a similarly sharp peak, reinforcing the observation of a homogeneous chemical composition of the epitaxial NiAl.

This strain-free epitaxial configuration is identified as a primary factor contributing to the significant reduction in compositional fluctuations, highlighting the advantages of such strain-free epitaxial intermetallics for advanced interconnect applications.

References
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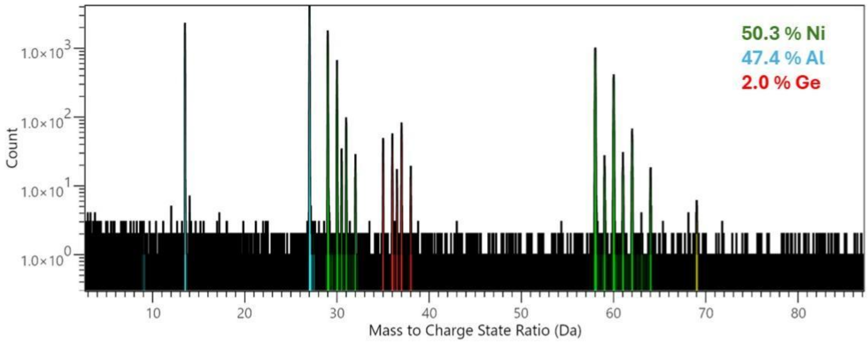

Figure 1: Mass to charge state ratio spectrum in the sub-cylindrical region.

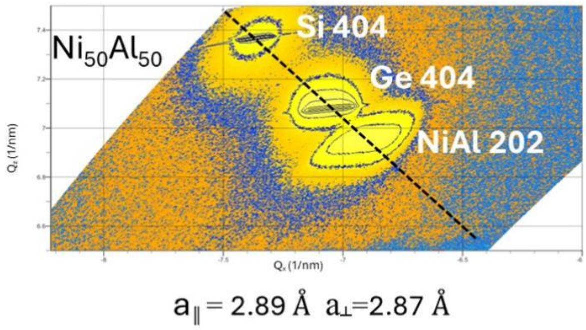

Figure 2: Reciprocal space mapping of Si (404), Ge (404) and NiAl (202).

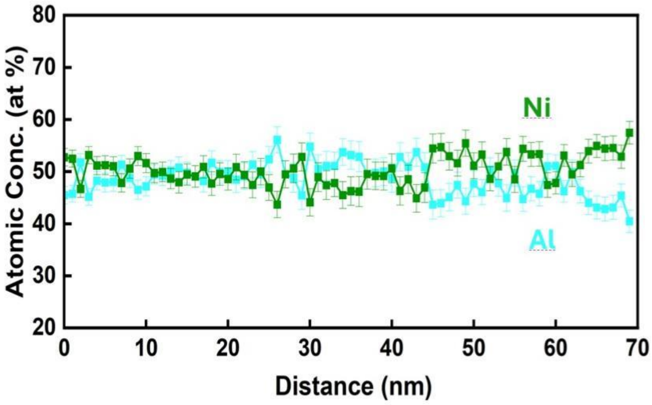

Figure 3: Atomic concentration distribution as a function of distance.

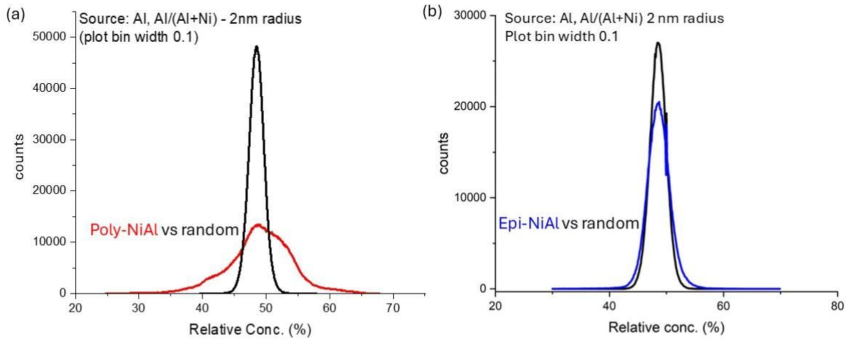

Figure 4: Measured relative concentration in the (a) polycrystalline and (b) epitaxial NiAl thin films compared with the randomly shuffled data.