A model for the redistribution of Pt during the agglomeration of Ni(Pt)Si thin films

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Silicides, particularly thin films of Ni-Pt monosilicide (Ni(Pt)Si), are widely employed as contact materials in microelectronic devices, especially in complementary metal-oxide-semiconductor (CMOS) technologies. Their popularity is due to several advantages, including low resistivity and high thermal stability. However, as device dimensions shrink, contact thickness requirements can be as low as 10 nm, presenting significant challenges.
At such small scales, Ni(Pt)Si films become highly susceptible to agglomeration during high-temperature processing [1,2]. This agglomeration, driven by the reduction of interfacial energies and controlled by diffusion, can lead to morphological discontinuities and significantly reduce device yield. In polycrystalline thin films, agglomeration typically begins with grain boundary grooving, and usually results in isolated islands. For NiSi films, these islands form within the silicon substrate rather than on its surface, a phenomenon known as inverse agglomeration [1]. Luo et al. have shown that the slow diffusion of Si at the silicide/substrate interface plays a crucial role in NiSi agglomeration [1].
The addition of Pt to NiSi has been found to delay agglomeration, shifting it to higher temperatures [3,4], and is thus used industrially to stabilize the low-resistivity NiSi phase during high-temperature processing. However, the precise role of Pt in the agglomeration process is not yet fully understood and warrants further investigation.

In this study, the redistribution of Pt during the agglomeration of Ni(Pt)Si films is investigated using scanning transmission electron microscopy with energy-dispersive X-ray spectroscopy (STEM-EDX) measurements (Fig. 1). Results indicate that agglomeration follows the classical steps, beginning with the formation of holes by grain boundary grooving, and finally the expansion of holes, resulting in isolated islands of Ni(Pt)Si. The surface of the sample remains flat, corroborating the particularity of inverse agglomeration in Ni(Pt)Si thin films (Fig. 1.a). Moreover, the complex redistribution of Pt is characterized by the existence of three different regions: a Pt-rich surface region, a Pt-depleted region within the grain, and a moderately Pt-rich region near the silicide/Si interface that corresponds to the displaced Ni(Pt)Si (Fig. 1.d). A model is developed to describe the redistribution of Pt during grooving and agglomeration. A model based on spherical cap geometry is developed to describe the redistribution of Pt during grooving and agglomeration (Fig. 3). It is based on similar assumptions to our previous model [1], with additional assumptions for the Pt redistribution including diffusion at the silicide/Si interface (Fig. 4). The model allows reproducing the Ni(Pt)Si island shape and Pt redistribution within these islands after grooving and agglomeration (Fig. 5) but underestimates the concentration of Pt in the displaced Ni(Pt)Si. The difference can be explained by diffusion from the Pt-rich sub-surface region to the region near the silicide/Si interface, involving volume diffusion in addition to diffusion at the surface, grain boundaries (GB), and interface, which are fast diffusion paths (Fig. 2). These findings have implications for understanding the complex nature of Ni(Pt)Si agglomeration and, especially, the role of Pt in the agglomeration phenomenon.

References

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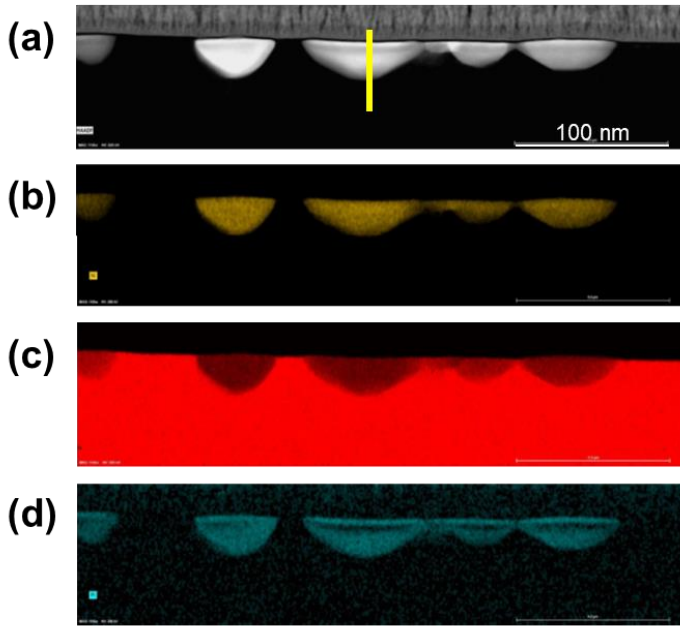
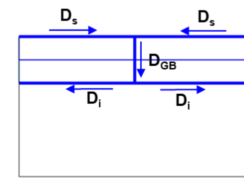
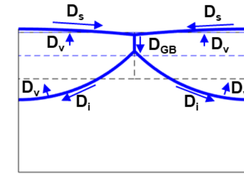


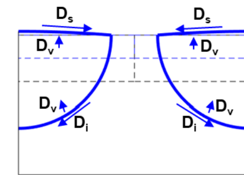
Figure 1: STEM-EDX cross-sections of the sample after the salicide heat treatment and RTAD at 700 °C: (a) STEM image, (b) Ni EDX map, (c) Si EDX map, and (d) Pt EDX map.



(a) Formation of NiSi



(b) grooving



(c) agglomeration

Figure 2: Schematics illustrating diffusion paths during different processing steps: (a) Formation (b) Grooving (c) Agglomeration

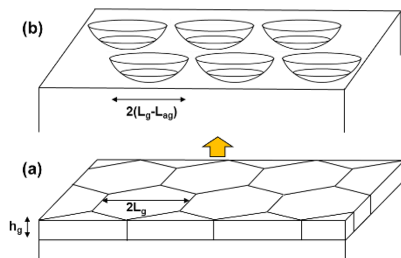


Figure 3: Schematics of the geometry used for the redistribution model: (a) initial columnar grains with a hexagonal base, (b) islands with a spherical cap shape after agglomeration

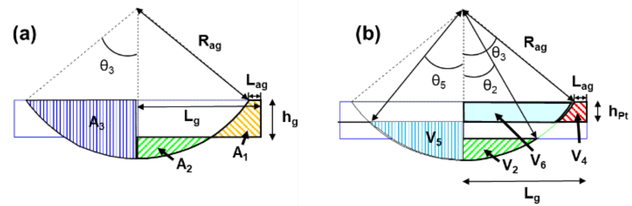


Figure 4: Schematic of the model used to simulate the agglomeration (a) change in the grain shape (b) redistribution of Pt. Only half of the annotated volumes is shown for clarity

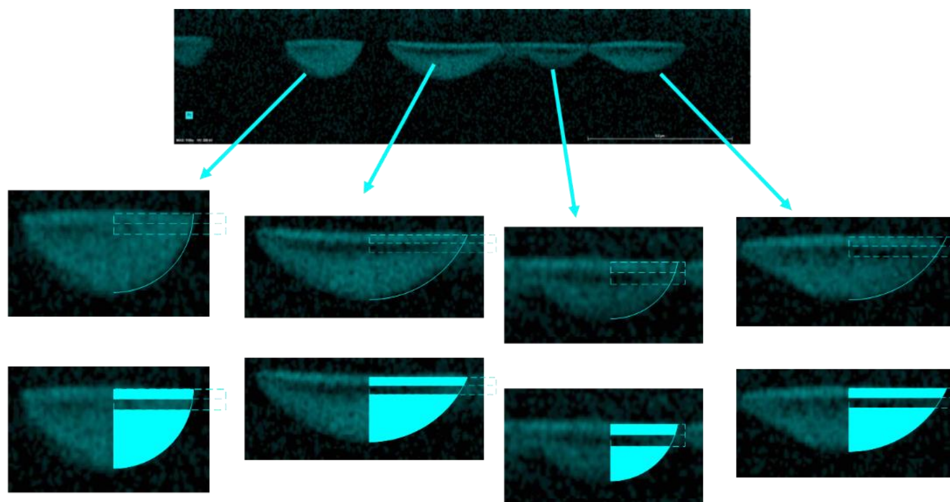


Figure 5: Fit of the EDX map for Pt for four grains after agglomeration (RTAD 700°C) using the present model: (a) whole EDX map for Pt, (b) EDX map for Pt with the fitted shape and Pt-rich region superimposed, (c) same as (b) with the Pt-rich regions highlighted in blue