

Geometry-dependent phase/stress and electrical resistivity in nickel-silicide nanowires

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Abstract

We report that purely the geometry of the Si nanowire (NW) can control the phase, stress state, and electrical resistivity of the Ni_xSi_y NW that is formed by silicidation of lithographically-patterned Si NWs at 500°C. A volume-accommodation mechanism is proposed to explain the observed width-dependence of Ni_xSi_y phases and electrical resistivity in NWs.

1. Introduction

Nickel silicidation, converting Si that is in direct contact with nickel into Ni_xSi_y following thermal anneal, has become the norm for fabricating ohmic nanocontacts within nano technology nodes thanks to the low process temperature, less silicon consumption, and good electrical conductivity. The key to successfully realizing high-performance nickel-silicide nanocontacts lies in the thermal stability of their material structure via desired phase formation. Therefore, the understanding of geometrical size and stress state effects on the morphological stability, phase formation, and electrical properties of Ni_xSi_y nanowires (NWs) is of high importance for creating reliable and reproducible Ni_xSi_y nanocontacts.

In this paper, we report that the geometric size of the Si NW can control the phase, stress state, and electrical resistivity of the Ni_xSi_y NW that is formed by silicidation of lithographically-patterned Si NWs at 500°C. A volume-accommodation mechanism is proposed to explain the observed width-dependence of Ni_xSi_y phases and electrical resistivities in NWs.

2. Experimental

The fabrication of Ni_xSi_y NWs started with the thinning-down of the top layer of c-Si in silicon-on-insulator (SOI) wafers. The top c-Si layer thickness was reduced from an initial thickness of 192 nm to two final thicknesses (H_f) of 75 ± 5 and 45 ± 5 nm using $\text{SF}_6/\text{C}_4\text{F}_8$ plasma etching. Rectangular-shaped Si NWs in width (W) of 40–500 nm and length of 2 μm were then generated using a combination of electron-beam lithographical patterning and plasma etching. Sequential processes of HF dip, thermal evaporation of Ni encapsulating layer over the c-Si NWs, rapid-thermal anneal at 500°C for 15 sec, followed by a wet chemical wash to remove unreacted nickel metal were conducted for the formation of Ni_xSi_y NWs (Fig. 1a). The thickness of Ni encapsulating layer was selected to be 45- and 75-nm in order to provide sufficient Ni for complete silicidation of the entire Si NW. Structural properties and electrical resistivity of nickel silicide NWs were characterized using scanning electron microscopy (SEM), transmission electron microscopy (TEM) and diffraction pattern analysis and current-voltage (I - V) characterization.

3. Results and Discussion

The interesting new result is that the ultimate phase, stress state, and electrical resistivity of the Ni_xSi_y NWs appear to be strongly influenced by the original c-Si NW geometry, i.e. width and thickness. Notably the silicidation of a Si NW at 500°C induces an anisotropic volume expansion that appears to be highly dependent on the initial width and thickness of as-formed Si NWs (Fig. 1b). Ni_xSi_y NWs not only expand vertically in thickness by a constant factor of 1.25 ± 0.1 for all experimental c-Si NWs (Fig. 2a), but their widths also have an inverse dependence on the width of the c-Si NWs (Fig. 2b). The overall volume expansion factor for Ni_xSi_y NWs to c-Si NWs ranges from 1.3 to 2.6 (Fig. 2c), apparently greater than the value of 1.2 for NiSi in the thin-film form. This experimental finding suggests Ni-rich phase

formation for the Ni_xSi_y NW in sharp contrast to the formation of nickel monosilicide for the NiSi film.

Concurrent with the inverse size-dependent volume expansion for Ni_xSi_y NWs, we also observe a unique undulation in electrical resistivity for the NWs ranging from 40–500 nm in width (Fig. 3). In particular, for given cases of the 45-nm-thick Ni encapsulating layers, the electrical resistivity for 200–450nm-wide Ni_xSi_y NWs retains a low, constant value at $25 \mu\Omega\text{-cm}$, while an unusual fluctuation in electrical resistivity was found when the Ni_xSi_y NW width is downscaled to 150 nm or even smaller. Another anomaly in electrical resistivity was further exemplified by the case of the 75nm-thick encapsulation Ni layers. The electrical resistivity appears to decrease with reducing the NW width from 450 to 150nm and then turns to increase when the NW width is less than 100nm.

The observed, interesting physical size expansion together with unusual electrical resistivity fluctuation when reducing the geometrical sizes of Ni_xSi_y NWs obviously differ from the consequence of the so-called “reversed fine line” effect.

The unique size-dependent volumetric expansion coupled with unusual electrical resistivity fluctuation behaviors suggests possible phase transition in Ni_xSi_y NWs. Our extensive TEM/selected area diffraction (SAD) examinations (more than 5 points for each NW) corroborate that phase formation in Ni_xSi_y NWs is not simply in nickel monosilicide NiSi state, instead, the phase formation is highly dependent on their original c-Si NW width, that is, the narrower the c-Si NW width, the higher Ni incorporation. Figure 4 shows that in the case of 75-nm-thick encapsulation Ni layer, NWs generated from 250–450-nm-wide c-Si NWs are in the NiSi phase, whereas Ni_2Si is preferred for smaller NWs in width of 70–100nm. The phase transition from NiSi for large NWs to Ni_2Si for small NWs is well correlated with the observed volumetric expansion dependency on the NW size.

We are able to further gain insights on the crystalline orientation relationship between Ni_xSi_y NWs and their original c-Si NWs from detailed SAD analysis. We observe that atomic planes $\{110\}$, $\{112\}$, and $\{011\}$ of 100–450nm NiSi NWs align well with $\{020\}$, $\{022\}$, and $\{011\}$ planes of their original c-Si NWs, respectively, when the zone axis $[-110]$ of NiSi NWs are in parallel with $[100]$ of c-Si NWs (Fig. 5). Also when the zone axis of $[-101]$ and $[-110]$ for 250–450nm NiSi NW and for 70–450nm Ni_2Si NWs, respectively, are in parallel with $[100]$ axis of the c-Si NWs, their atomic planes of $\{111\}$, $\{010\}$, and $\{101\}$ are in good alignment with $\{020\}$, $\{011\}$, and $\{011\}$ of c-Si NWs, respectively. Figure 5 further reveals that for the c-Si NWs greater than 100nm in width, the diffraction spots appear to have a good match for NiSi NWs and c-Si NWs, whereas deviations in diffraction spots between 100nm-wide Ni_2Si NWs and c-Si NWs appear and greater local lattice deformation is observed for 70nm-wide NWs. Figure 6 shows simulated atomic structures of c-Si NWs, NiSi and Ni_2Si NWs. There appears to be a tensile stress in the NiSi and Ni_2Si NWs during the silicidation of c-Si NWs, and the strain value is enhanced from -0.4% through 3.2% to 6.4% by reducing the NW width from 450nm through 250nm to 100nm. Armed with the knowledge gaining from extensive TEM and SAD analysis, we believe that the presence of solely NiSi phase formation for the larger NWs (>100nm-wide) is attributable to the fact that the wide, rigid c-Si NW tightly-bound to the SOI substrate cannot deform themselves plastically for accommodating more Ni within its lattice. This leads to the NiSi grains being in a state of high elastic stress. When Si NWs are narrow, for instance, 100 nm in width or below, they are less resistive for interstitial diffusion of Ni and can accept higher content of Ni,

resulting in the formation of Ni_2Si or Ni-rich silicides. Also the less rigid Si NWs are capable of accommodating very large lateral deformations through plastic deformation, and hence primarily low elastic stress is observed in conjunction with the presence of higher density of small Ni_2Si poly-grains.

4. Conclusions

We reported that purely the geometry of the Si NW can control the phase, stress state, and electrical resistivity of the Ni_xSi_y NW that

is formed by silicidation of lithographically-patterned Si NWs at 500°C . We envisage further scientific exploration of the NiSi NWs as a building block of the nanoelectronics for ULSI technology.

Acknowledgements

This work was supported by the Ministry of Science and Technology of R. O. C. (MOST102-2221-E-009-195-MY3) and US Air Force (FA2386-15-1-4025).

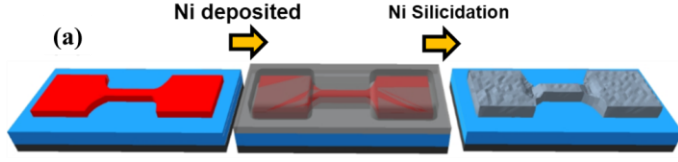


Fig. 1 (a) Schematic diagram of Ni_xSi_y NW generation and (b) Cross-sectional SEM micrographs of Si NWs before and after Ni silicidation.

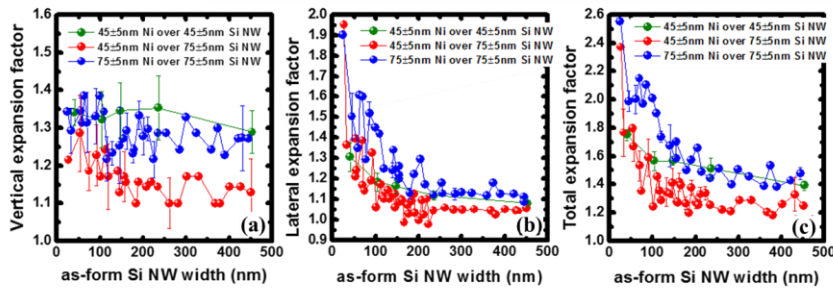
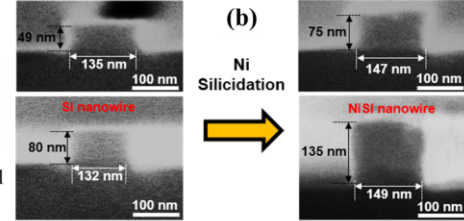


Fig. 2 (a) Lateral, (b) vertical, and (c) total volume expansion of Ni_xSi_y NW relative to original Si NW.

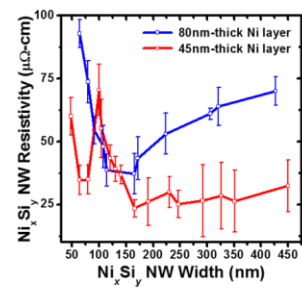


Fig. 3 Size-dependent electrical resistivity of Ni_xSi_y NWs.

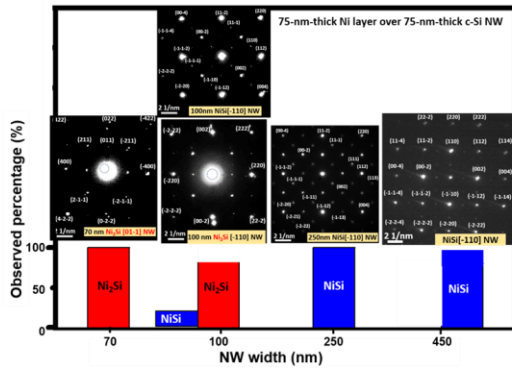


Fig. 4 Representative phases formation and in Ni_xSi_y NWs of various widths.

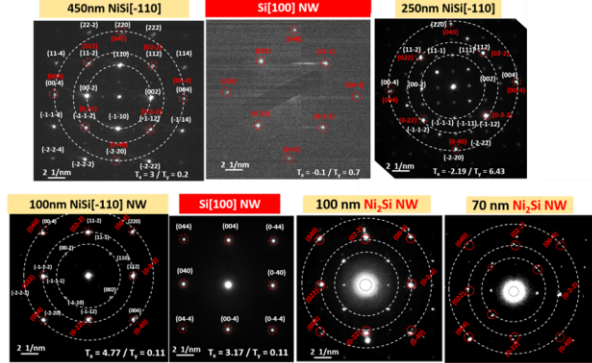


Fig. 5 SAD of Ni_2Si and NiSi NWs generated from 70-450nm-wide c-Si NWs after RTA at 500°C for 15sec.

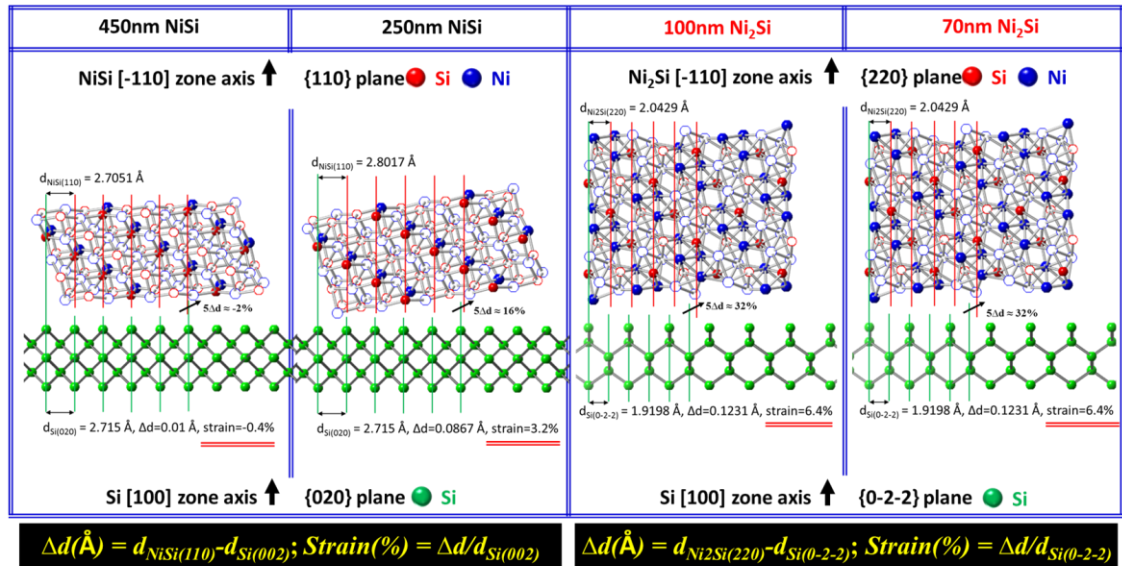


Fig. 6 Simulated atomic structures of Si NWs as well as NiSi and Ni_2Si NWs with zone axis of [100] and [-110], respectively.