## **Supplementary materials**

# Dependence of Structure and Orientation of VSS grown Si nanowires on Substrate Lattices

Yi-Ting Chiang, Yi Chou, Chang-Hsun Huang, Wei-Ting Lin, and Yi-Chia Chou

### 1. Geometry of Si samples

The Si substrates were diced from Si (111) wafer to rectangular blocks with dicing along the primary flat (110) of the Si(111) wafer (Fig. S1). So the rectangular blocks with (111) surface and (110) surface were obtained for observation of growth on both (111) and (110) surfaces.



Figure S1. Illustration of sample geometry from wafer dicing.

#### 2. Ni silicide formation

Annealing of Ni depositing on Si substrates leads to Ni silicide formation. The phase sequence starts from Ni-rich phase to Si-rich phase. It is in agreement with our experimental observation that the final phase is NiSi<sub>2</sub>, which acts as catalyst for further Si nanowire growth. In addition, from the phase diagram, it shows that most Ni silicide phases are intermetallic compounds. It suggests that the growth is mediated by vapor-solid-solid mechanism, where SiH<sub>4</sub> is vapor, NiSi<sub>2</sub> catalyst is solid, and the grown nanowire is solid.



Figure S2. Binary phase diagram of Ni and Si.<sup>1</sup>

## **3. Define growth orientation**



**Figure S3.** Stereographic projection related to the [111] orientation. The degrees on each circle indicate the angle to the [111] direction.<sup>2</sup>

In order to identify the growth directions in Fig. 2d and e, stereographic projections

(Fig. S3) with respect to the [111] direction were utilized. It illustrates that the nanowires grown on Si (111) followed <112> and <110> directions.

Fig. S3 illustrates the stereographic projections of low-index orientations of cubic crystals generated from the fact that the most observed growth directions are <111>, <110> and <112> family.<sup>2</sup> The degrees on each circle indicated the angles to the [111] direction in three-dimensional space.

#### 4. Twinning in large Si nanowires

The twinning in nanowires has been repeatedly seen in the experiments. Another examples of Si nanowires with twin interface along the axial direction were added as Fig. S4. The Fig. S4a represents the larger nanowires with tip shape identical to Fig. 3f where the twin interfaces are along the axial direction. Fig. S4b and c are TEM and HRTEM images of the nanowire. The nanowire shown in Fig. S4b may be inclined or the suffer from T change to affect the interface morphology. Note that such nanowires are less and shorter so we did not find many larger ones after they were randomly scratched onto the TEM grid.



**Figure S4.** SEM and TEM images of nanowires with diameters larger than 100 nm. (a) SEM images of Si nanowires, where the larger ones were indicated by white circles. (b) Another enlarged image of a nanowire with twin interface. (c) HRTEM image taken at the twin interface.

#### 5. Effect of temperature and precursor gas flow

In the experiments, the growth T was 400 °C, where we found that at the T higher than it (say 450 °C) the nanowires tended to grow widely. They stopped growing at even higher T (T > 500 °C). If the T went lower than 400 °C, the decomposition of silane was too inefficient and limited which lower the growth rate. So we chose 400 °C as the growth T to remain in growth zone and to achieve reasonable growth rate that is not too slow during 1 hr growth.

In previous reported nanowire growth in ultra high vacuum system, some nanowires frustrated when they were short (Ref. 15 in main text) and the growth rate of nanowires

was proportional to the amount the precursor gas<sup>3</sup>. Based on the understanding, we just selected high growth pressure to achieve higher growth rate and obtain straight and long nanowires but did not spend time on exploring growth at lower pressure, which benefit to further property measurements and evaluation for applications.

## 6. STEM EDS analysis of Si and GaN interface

The atomic distribution of Si and Ga have been analyzed using STEM EDS.



**Figure S5.** STEM EDS analysis at the interface of GaN and Si. (a) STEM image taken at the interface of GaN and Si. The inset is the FFT where yellow line marked the low index diffraction spots and blue one for Si. (b) STEM EDS mapping at the interface show Si and Ga atoms distribution.

Reference:

- 1. Connetable, D.; Thomas, O. J. Alloys Compd. 2011, 509, 2639-2644.
- 2. Schmidt, V.; Wittemann, J. V.; Gosele, U. Chem. Rev. **2010**, 110, 361-388.
- Wen, C.-Y.; Tersoff, J.; Hillerich, K.; Reuter, M.; Park, J. H.; Kodambaka, S.; Stach, E. A.; Ross, F. M. Phys. Rev. Lett. 2011, 107, 025503.