Electronic Supplementary Material (ESI) for Nanoscale.

Unique features of laterally aligned GeSi nanowires self-assembled on the vicinal Si (001) surface misoriented toward [100] direction

Tong Zhou,[a] Guglielmo Vastola,*[b] Yong-Wei Zhang,*[b] Qijun, Ren,[a] Yongliang Fan,[a] Zhenyang Zhong*[a]

[a] State Key Laboratory of Surface Physics and Department of Physics, Collaborative Innovation Center of Advanced Microstructures, Fudan University, Shanghai 200433, China

[b] A*STAR Institute of High Performance Computing, 1 Fusionopolis Way #16-16, Connexis, Singapore 138632

*Corresponding Author: vastolag@ihpc.a-star.edu.sg; zhangyw@ihpc.a-star.edu.sg; zhenayngz@fudan.edu.cn

Raman characterization

Raman spectra from the single layer of GeSi nanowires (NWs) are rather weak due to the quite small size of the NWs. Accordingly, ten layers of GeSi NWs with Si spacers are employed for Raman characterization. In each layer, 5.4 momolayers (ML) Ge are deposited at 515 ºC, which is separated by 25 nm Si. To suppress the Ge segregation during the Si spacer layer growth, the first 5 nm Si are grown at 400 ºC. Then additional 20 nm Si are grown with ramping the growth temperature from 400 ºC to 550 ºC. Considering the relatively thick Si spacer with respect to the size of NWs, we argue that the GeSi NWs in each layer of the multilayer sample are essentially independent. In other words, the size and the Ge composition of NWs in each layer are nearly the same. This argument is supported by Figure S1 (a), which shows the surface morphology of the 10^{th} layer of GeSi NWs. It can be seen that the size of NW is not so much different from the case of single layer. The micro-Raman spectra are performed by using a Horiba LabRam HR spectrometer. The incident laser light with a wavelength of 532 nm is focused on samples in diameter of ~1μm. The spectral resolution of the spectrometer is about 0.5cm^{-1}. The Raman spectra from the ten layers of samples are shown in Figure S1 (b). It can be clearly seen that the Raman spectra from the GeSi NWs on different miscut Si (001) substrates are nearly the same. This means that the Ge composition in NWs is essentially not affected by the miscut angle. The Ge-Ge and Si-Ge modes form GeSi NWs are observed at ~302 cm^{-1} and ~416 cm^{-1}, respectively. The frequencies of these two modes can be estimated by the follow formula,[1]

$$\omega^{Si-Si}(x,\varepsilon) = 520.7 - 66.9x - 730\varepsilon$$
$$\omega^{Si-Ge}(x,\varepsilon) = 400.1 + 24.5x - 4.5x^2 - 33.5x^3 - 570\varepsilon$$

Where x is the Ge content in GeSi NWs, ε is the strain of GeSi NWs. By fitting the data, we obtain the Ge composition in the NWs to be ~66%.

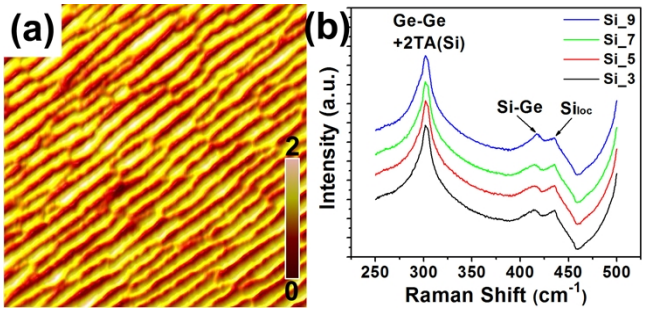

Figure S1. (a) AFM images ($0.5\times0.5\mu m^2$) of the surface morphology of the 10th layer of GeSi NWs on Si (001) /[100] 7º. (b) Raman spectra of the ten layers of GeSi NWs on Si (001) /[100] θ(θ=3º, 5º, 7º, 9º) substrates.

Details on the surface energy parameterization

In Eq.(1) of the paper, the analytic expression for the surface energy as a function of both the miscut angle and the film thickness was reported. Here, we further explain how the numerical values for γ were derived, based on the ab-initio calculations of Citation [33] in the manuscript. By choosing a value for the film thickness, in units of (001) ML we calculated the values for the surface energy of the (001) and (105) orientations following the procedure in [33]. Later, these two values were set as constrains for our surface energy function Eq. (1). In this way, a set of parameters for a specific film thickness was obtained. For example, parameterization of γ for Ge film thickness of 0ML is shown in Fig. S2. From the figure we can see that the energy difference between the (001) and (105) orientation is very small, obviously in agreement with [37]. After a set of parameters was obtained for a specific film thickness, the procedure was iterated to get the parameterization at every other film thickness, up to 4 (001) MLs. This procedure, ultimately, allows us to reproduce the data shown in Figure 6 of the paper.

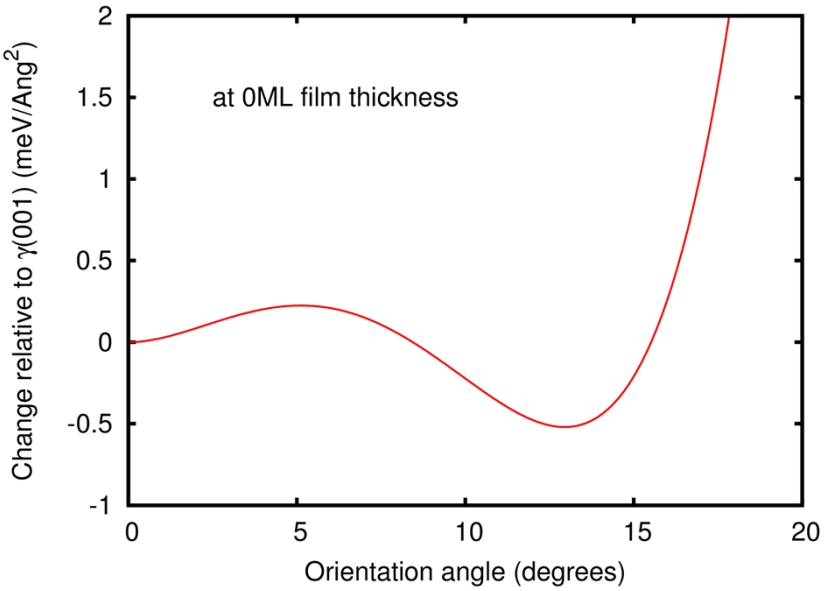

Figure S2. Explicit plot of the surface energy for the case of 0 (001) ML film thickness (a bare Silicon substrate). The difference between (001) and (105) surface energy is very small at this film thickness, in agreement with Ref. 37.

REFERENCES

1. Pezzoli, F.; Bonera, E.; Grilli, E.; Guzzi, M.; Sanguinetti, S.; Chrastina, D.; Isella, G.; von Känel, H.; Wintersberger, E.; Stangl, J.; Bauer, G. *Materials Science in Semiconductor Processing* **2008,** 11, 279-284.