	Experiment title: Structural X ray diffraction investigation of silicon nanowires growth in a porous alumina template	**Experiment number**: 02-02-733
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Report:

Aim of the experiment :

The aim of this experiment is to perform an *ex-situ* structural characterization of silicon nanowires (SiNW), grown on a <111> orientated silicon substrate under catalytic conditions. Before the nanowire growth, the catalyst (Gold (Au) was deposed by evaporation, following by a dewetting under high temperature resulsting in a assembly nanometric dropplet. Next, the growth of nanowires onto a silicon substrate by Vapor-Liquid-Solid method under a Chemical-Vapor-Deposition mode, lead an assembly of crystalline silicon nanowires which much ne investigated. This is supposed to yield important knowledge about the growth characteristics like epitaxial and crystalline properties, lattice parameter, strain, defects and shape/faceting of the SiNW.

Measurements :

We have performed the lattice mismatch parameter measurements between (SiNW) and the silicon substrate. The selected energy was $E = 11.4$ keV corresponding to a wavelength $\lambda = 0.108758$ nm. The experimental set-up was a 7-circles goniometer, and the detector was a punctual NaI scintillator. Three samples were investigated of three different length L: short (S), medium (M), long (L) wires (resp. $L = 350, 1177, 2782$nm).

Results :

We have performed Grazing Incident X Ray Diffraction (GIXD) measurements. Typical profiles of diffraction are shown on Figure 1. The diffracted intensity is plotted versus the scattering vector q along the in-plane direction <300> (of the hexagonal system) for the <111> oriented silicon wafer. The profile reveals a narrow peak (Sub) coming from the diffraction by the silicon substrate, and also a broader one (SiNW) which is attributed to the Bragg's diffraction of the silicon nanowires. This observation gives evidence of the

crystalline character of the wires, and also of their epitaxy with the silicon substrate. Even if the peak is broader than the substrate, it is relatively narrow and well defined. There is only a small mosaicity in the wires and only a very few defects. Both peaks (SiNW) and (Sub) have different q values. In consequence there is a lattice mismatch parameter $\Delta a/a$ between the silicon wafer and the silicon nanowires (defined by: $\Delta a/a = (a_{SiNW}-a_{Sub})/a_{Sub}$, where a_{SiNW} and a_{Sub} are the lattice parameter of the silicon nanowires and of the substrate respectively). As we see Figure 1, $q_{SiNW} < q_{Sub}$, which evidences that $\Delta a/a > 0$.

We present in Figure 1 results of profiles of diffraction by varying the incident angle close to the critical angle α_c. For short wires (S) and for α_i close to 0°, we observe only one peak (SiNW). As the angle of incidence α_i increases, a narrow peak of diffraction appears at the right of the (SiNW) peak. For $\alpha_i = \alpha_c$ this narrow peak become very intense, and then we attribute this peak to the diffraction of the x-ray beam by the silicon substrate. As the wires are very short, when α_i increases, the cross section of the beam with the sample decreases and the intensity of (SiNW) decreases, also observed for $\alpha_i > \alpha_c$ (Figure 1 (b)). For long wires (L), Figure 1 (c) shows similarly behaviour. We present in Figure 2 the evolution of the in-plane lattice mismatch parameter Δa/a versus the length of nanowires along the radial <300> direction (full circles). The in-plane $\Delta a/a$ is positive corresponding to a small expansion of the crystalline lattice of SiNW. As it can be seen the $\Delta a/a$ is close to $+5.2\times10^{-4}$ when the length of the wires $L > 1000$ nm, while for shorter nanowires $\Delta a/a \approx +3.4\times10^{-4}$. The $\Delta a/a$ along the in-plane perpendicular direction was also measured and is reported by full triangles. Consequently the expansion is similar and the strain is symmetrical in agreement with the symmetrical character of the cylindrical wires.

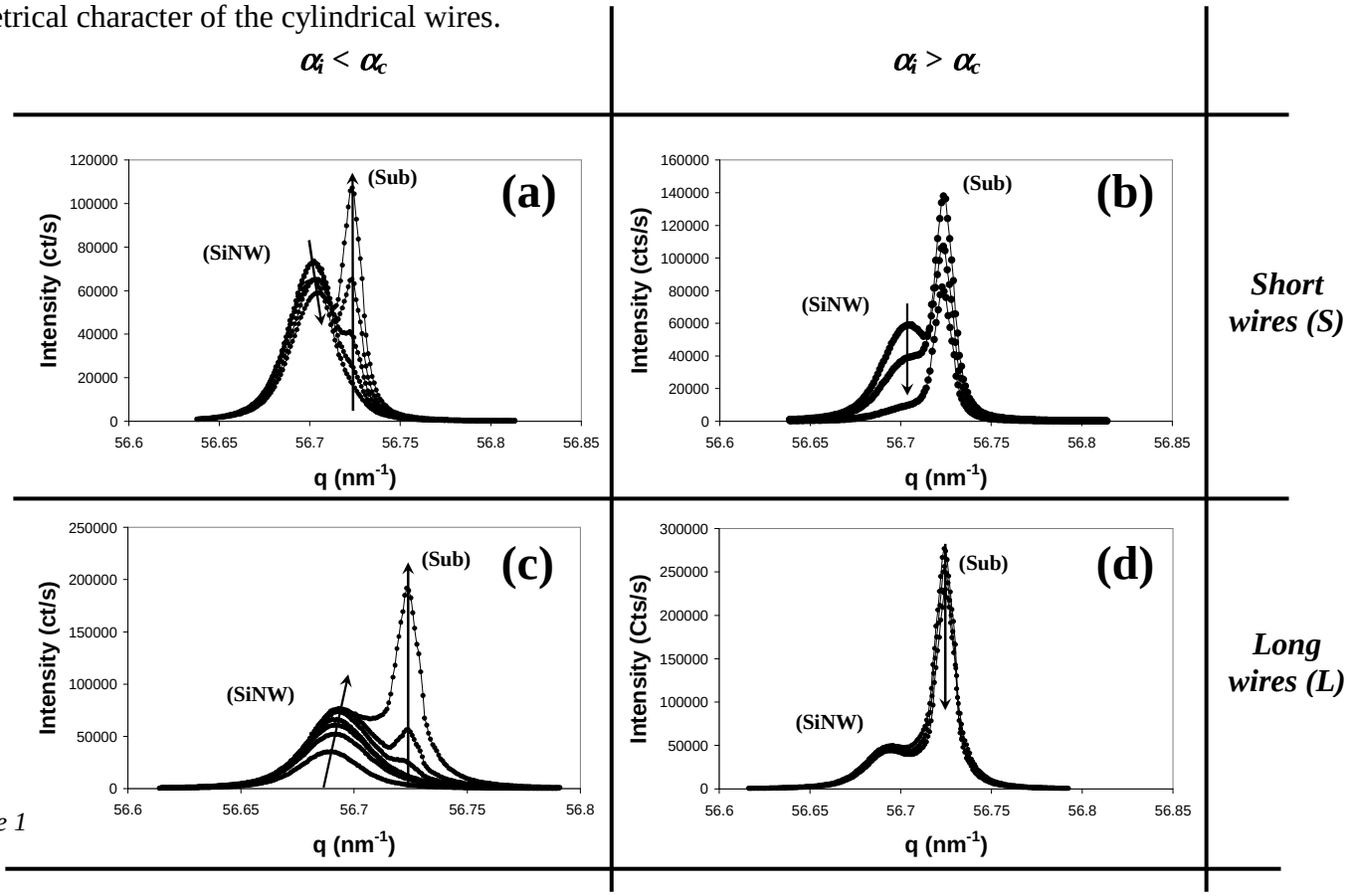

Figure 1

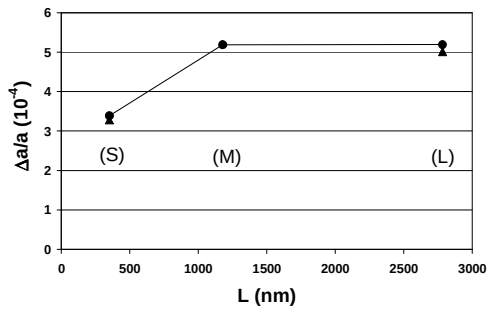

Figure 2

Conclusion

In conclusion, we have investigated, the lattice mismatch parameter $\Delta a/a$ between the Silicon substrate and the SiNW and give evidence that the SiNW are in expansion. This expansion as been measured versus the incident angle and the SiNW lentgh. The presence of gold (Au) could explained this expansion and will be investigated in a further experiment.