ESRF	**Experiment title: Influence of faceting and catalyst on the lattice mismatch parameter of silicon nanowires grown by catalytic VLS method**	**Experiment number**: 02-02-759
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Shifts: 9	**Local contact(s)**: Jean-François Bérar	*Received at ESRF:*

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Report:

Aim of the experiment :

The aim of this experiment is to continue previous experiments (02-02-733) devoted to *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. The aim of this experiment is to investigate the influence of the gold catalyst onto the lattice mismatch parameter.

Measurements :

We have performed the lattice mismatch parameter measurements between (SiNW) and the silicon substrate. The selected energy was $E = 12.2$ keV corresponding to a wavelength $\lambda = 0.101837$ 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 (full circles). 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 $\Delta a/a > 0$.

In order to understand the origin of the SiNW expansion we have performed measurements after removing gold catalyst by dipping all the samples successively 3 solutions: HF, HNO_3-HCl, HF. GIXD measurements with such samples were performed and also reveal a Bragg diffraction peak (SiNW) show in Figure 1 (open circles). In order to compare both measurements before and after the gold removing we have plotted two profiles of diffraction. The profile with the full circles corresponds to the sample with gold and the one with open circles corresponds to the sample without gold. The shape of the profile is similarly to the one obtained before with gold. The (Sub) peak is narrow and the (SiNW) one is slightly broader.. We observe a small shift of the (SiNW) peak to the higher q values which corresponds to a small decrease of the lattice expansion. This measurement was perform for all the samples and is plotted in Figure 2. The in-plane $\Delta a/a$ along the <300> direction is reported with open circles. We find a curve with a similar shape than the one with gold, with a small decrease of the in-plane $\Delta a/a$ for small nanowires (S). All values decrease by a constant $\approx 0.9\times10^{-4}$. The measure along the perpendicular direction is reported with open triangles and reveals the same value. This confirms the symmetrical character of the strain. At last we have performed measurements of in-plane $\Delta a/a$ by varying the incident angle for $\alpha_i < \alpha_c$ (Figure 3 open circles and triangles). We observe a small shift of the $\Delta a/a$ value, which evidence that $\Delta a/a$ is smaller close to the substrate than the top.

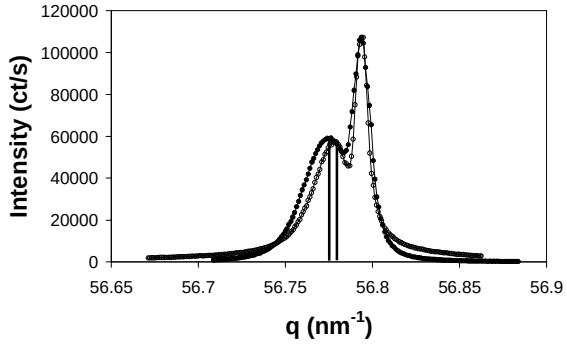

Figure 1

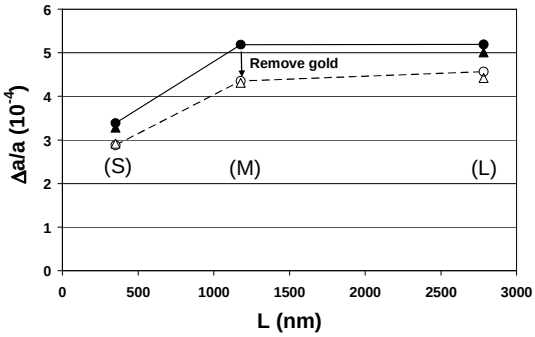

Figure 2

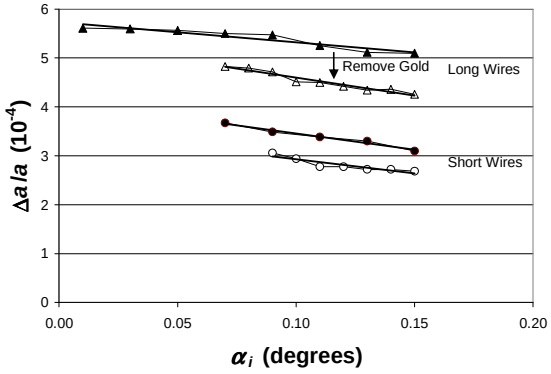

Figure 3

Conclusion

In conclusion, small in-plane positive lattice mismatch parameter $\Delta a/a$ of few 10^{-4} between silicon nanowires and bulk silicon substrate was experimentally measured by GIXD, and corresponds to small in-plane expansion of the nanowires (i.e. along and normal to the <300> direction). The influence of the gold catalyst is measured and clearly demonstrated.