JOURNAL OF APPLIED CRYSTALLOGRAPHY

Volume 49 (2016)

Supporting information for article:

Quasi-fivefold symmetric electron diffraction patterns due to multiple twinning in silicon thin films grown from hexamethyl-disiloxane

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S1. Chemical analysis

Elemental maps of silicon, carbon and oxygen were performed, using energy-filtered TEM (EFTEM), on samples deposited with an HMDSO flow rate of 0.45 sccm on Si (100) with epitaxial film/substrate interface. The concentrations of these elements were quantified by correlating EFTEM and secondary ion mass spectrometry (SIMS) measurements expressed as arbitrary units and atoms/cm^3, respectively. Given that the bulk of the substrate does not contain oxygen and carbon before TEM sample preparation, and that its oxidation (or contamination) occurs on the TEM foil surfaces after sample preparation, we considered the bulk of the substrate as the level of contamination with carbon and oxygen. In order to have accurate elemental concentrations in the film, we first subtracted this contamination level, assuming that it is happening identically in the bulk of the film and in that of the substrate, and then we set the average value of the elemental profile in the bulk of the film as the average value of SIMS measurement in the same region.

A lack of silicon atoms at the interface manifests itself as a dark contrast in the silicon map Fig S1(a)), and a smaller concentration of silicon in HMDSO layer with respect to that of the wafer is also observed. In the oxygen map ((Fig S1(b)), the presence of a white thin oxygen-rich layer at the interface shows that the native oxide of the wafer was not completely etched. This interfacial oxide layer is presented by a peak in the profile of oxygen ((Fig S1(d)) having a concentration of ~ 8.4×10^{21} oxygen atoms/cm^3. A non-negligible amount of oxygen is found in the film and is estimated at ~2×10^{21} at/cm^3. In the carbon map (Fig S1(c)), we see no obvious contrast between the wafer and the film, but the profile of carbon ((Fig S1 (e)) shows the existence of ~2×10^{21} carbon at/cm^3 in the film. A small peak in this profile is present at the interface, which might be caused by carbon contamination of the surface of the wafer before deposition. At this point, we can explain the lack of silicon at the interface by a higher concentration of carbon and oxygen (impurities) atoms at this interface compared to these concentrations in the bulk of the wafer. It should be noted that the thickness map of the film, deduced from the ratio of the total beam intensity over that of elastically scattered electrons, indeed appeared constant with no fluctuations, suggesting that the missing silicon atoms had been replaced by other elements.

It is important to note that the presence of oxygen and carbon in the film comes from the use of the HMDSO precursor which contains one oxygen atom and six carbon atoms per HMDSO molecule. We showed in previous work (Goyal *et al.*, 2016) that when increasing the flow rate of HMDSO, there is more carbon and oxygen incorporation in the film, which causes a decrease in the crystalline fraction and explains the trend of Fig. 3. However and quite remarkably, whatever the flow rate of HMDSO precursor, carbon and oxygen are incorporated in about equal concentrations (Goyal *et al.*, 2016) and the ratio of the multiply twinned part to microcrystalline part is kept unchanged as we have demonstrated in section 3.4.

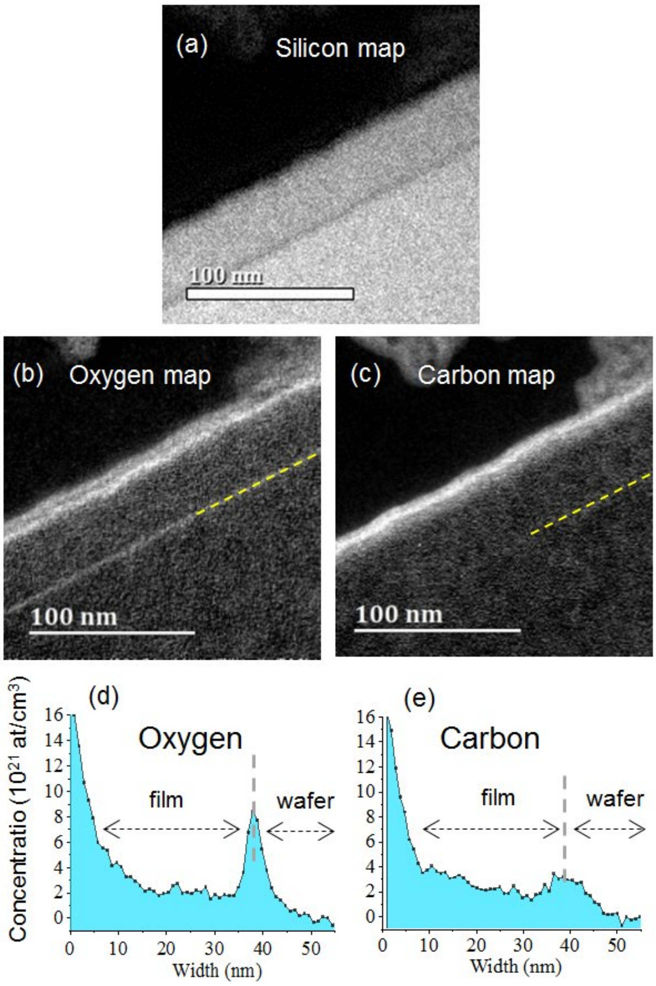

Figure S1 Elemental maps of silicon (a), oxygen (b) and carbon (c). (d) and (e) represent the profile of oxygen and carbon, respectively.

References

Goyal, P., Hong, J., Haddad, F., Maurice, J.-L., Cabarrocas, P. R. i. & Johnson, E. (2016). *EPJ Photovolt.* **7**, 70301.