Abstract for 3rd RMC

Possibility of the Reverse Monte Carlo Modeling for the Amorphous Si Deposited on the Reactive Ion Etched Si Substrate

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Amorphous Si (a-Si) was widely used for devices such as a thin film transistor and a solar cell. However, the precious sturdy for a materials with well worked device parameters are also required for the future high performance devices, as the amorphous materials generally has many structural freedom that can generate the many possible atomic configurations in the materials. Another aspect of the structural analysis for a-Si is that several deposition techniques such as cat-CVD and PE-CVD can fabricate the different structure in a-Si, which are usually classified by the hydrogen concentration. However, the 3D modeling for these structures seems to be important. Reverse Monte Carlo (RMC) modeling can generate the 3D modeling of the materials from the diffraction spectra without any internal potential.

X-ray diffraction is a powerful technique for the structural analysis and small amounts of the materials can be used comparing to the neutron diffraction and so forth. We have applied XRD for a-Si thin films deposited on the Si substrate. However, when the X-ray energy increases, the penetration of the X-ray prevent the high Q measurements of the materials for thin film samples, where the substrate signals should hide the main signals from thin films. On the other hand, real sample structures depends on the substrate, then the structural analysis for the thin film samples, should be done on the substrate.

So, we tried to measure the XRD for a-Si including the Si substrate in high Q measurements. In that case, to reduce the substrate signals, we should use the very thin substrate. To keep the free standing structures, the small area of the substrate was etched by the plasma process of reactive ion etching (RIE), and the a-Si was deposited by the aat-CVD techniques. The X-ray beam was focused on the etched area and a-Si diffraction with a thin Si layer was measured.

In the diffraction pattern for a-Si deposited on the Si substrate without etching, only the signals from Si substrate are observed, because the tail of the Si peaks hides the diffraction from the a-Si. Comparing to this, we are succeeded in the observation of the amorphous signals from the samples deposited on the processed substrate. Then, we discuss about the possibility of the RMC modeling using this data, subtraction of the Si substrate peaks.