Nucleation Mechanism of Microcrystalline Si from Amorphous Phase

We have characterized surface structures of hydrogenated amorphous silicon (a-Si:H) by applying infrared spectroscopy, in order to investigate the phase transition from a-Si:H to microcrystalline silicon (μc-Si:H). At the onset of μc-Si:H nucleation from the a-Si:H phase, an infrared absorption peak at 1937±5 cm⁻¹ assigned to the SiHₙ (n=1~2) complex is detected. The SiHₙ complex concentration within the a-Si:H surface region showed a clear relationship with the μc-Si:H nucleation. We confirmed that the SiHₙ complex, formed by insertion of H into a strained Si bond, contributes to the reactions that result in μc-Si:H nucleus formation.

New Theory for Photoinduced Phase Transitions in Nanostructures

By means of Monte Carlo simulations on a kinetic model, we demonstrate that the efficiency of a photoinduced phase change can in general be enhanced drastically by using a superstructure of an appropriate combination of two components. This is due to the accelerated nucleation of converted domains in the structural blocks relatively close to local instability. The present mechanism provides a general guideline on the design of photocontrollable materials with potential applications for memory and storage devices.