MASTER'S THESIS

Effect of thermal annealing on Si-H bonds and dangling bonds in amorphous silicon

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ABSTRACT

Amorphous silicon (a-Si) is a technologically important semiconductor in its hydrogenated form. It is believed that a hydrogen atom may interact with a dangling bond to form a Si-H bond and thus removes a corresponding trap level from the energy gap and improves material quality. However, hydrogenated amorphous silicon (a-Si:H) suffers from the well-known light-induced degradation or Staebler-Wronski (SW) effect. The SW effect involves the creation of light-induced metastable silicon dangling bonds with midgap electronic states under prolonged illumination. Hydrogen is suspected to play an important role in the formation and annihilation of the light-induced silicon dangling bonds. Several microscopic models for explaining the degradation were proposed but no model is satisfactory. In this work, a related problem was studied. In stead of studying a-Si:H under strong light illumination, the effect of thermal annealing on Si-H bond density and dangling bond density in a-Si thin film were investigated.

Amorphous silicon thin films were produced by radio frequency (RF) magnetron sputtering. X-ray diffraction patterns of the films show that the structure of the films was amorphous. Local vibrational modes of chemical bonds between Si atom and other impurities such as H and O in the a-Si films were studied by means of fourier transform infrared spectroscopy. The densities of the chemical bonds were calculated. The dangling bond density in a-Si films was measured by electron spin resonance spectroscopy as well.

It was found that the density of Si-H bond dropped from about 5 x 10^{18} cm^{-3} to an insignificant value when the film was annealed successively at temperatures from 20 °C to 800 °C. Near-infrared absorption corresponding to transitions between band tail states and gap states was found to increase with decreasing Si-H bond density. The results were interpreted in terms of dangling bonds in silicon.

The dangling bond density was also found to vary with the annealing temperature ranging from 20 °C to 950 °C. Detail analyses of the results were done. Attempts had also been made to relate these results to the various models for the creation of dangling bonds in silicon.

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