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TRANSPORT PROPERTIES OF μc-Si:H FILMS PREPARED BY VERY HIGH HYDROGEN-DILUTED SILANE PLASMA*

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Highly hydrogen-diluted silane plasma is used to fabricate microcrystalline silicon films in a plasma-enhanced chemical vapour deposition system. X-ray diffraction and micro-Raman scattering spectroscopy are utilized to characterize their microstructure properties. Dark conductivity and drift mobility are measured by the travelling wave method. With the decreasing gas flow ratio of silane-to-hydrogen from 2% to 0.2%, the crystalline volume fraction and the drift mobility increase at room temperature. Meanwhile, the dark conductivity increases initially and then decreases. The relationship between the microstructures and transport properties is discussed.

Keywords: Microcrystalline silicon; conductivity; mobility; travelling wave method
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I. INTRODUCTION

Hydrogenated microcrystalline silicon (μc-Si:H) is a new kind of material in thin-film technology and is widely utilized in thin-film devices, such as solar cells, flat-panel displays, and so on.[1] With the improvement in the well-established hydrogenated amorphous silicon (a-Si:H) technology, high-quality μc-Si:H films can be prepared in a plasma-enhanced chemical vapour deposition (PECVD) system. Compared with a-Si:H, a stronger absorption in the near-infrared region and improved electrical properties, such as dark conductivity and drift mobility, have been observed in μc-Si:H thin films.

In the past decades, much research work has been done to investigate the microstructures and transport properties of μc-Si:H thin films.[2,3] Tsai[4] reported the transition from amorphous to microcrystalline, which was due to the preferential etching of the amorphous phase by hydrogen plasma. Le Comber *et al.*[8] used the model, in which there were potential barriers in grain boundaries where the defects trapped electrons and through which the electrons could not transport easily, to discuss the relationship between microstructures and transport properties. But the mechanism of the charge transport, to our knowledge, still remains unclear. In this paper, X-ray diffraction (XRD) and micro-Raman scattering spectroscopy are used to investigate the microstructures of μc-Si:H films prepared with various ratios of silane plasma diluted by hydrogen ($R = [SiH_4]/[H_2]$) in a PECVD system. The transport properties of μc-Si:H films are investigated using travelling wave (TW) method which is different from the Hall measurement.[5] We focus our attention on the change of transport properties induced by hydrogen-diluted silane plasma.

II. EXPERIMENT

A set of μc-Si:H thin-film samples were deposited on quartz substrates heated at 350°C in the PECVD system. In the gas mixture of silane (SiH_4) and hydrogen (H_2), the flow rate of SiH_4 was kept at 1 sccm and the flow rate of H_2 varied from 50 to 500 sccm. We kept the chamber pressure constant at 67 Pa when the films were deposited. The thickness of the samples was about 1μm.

XRD and Raman scattering were used to characterize the structures of the μc-Si:H films. From XRD patterns, the crystalline orientation and grain sizes (D) can be obtained. The crystalline volume fraction (f_c) can be calculated from the Raman spectra. The transport properties such as dark conductivity (σ_d), drift mobility (μ_d), conductivity activation energy (E_σ) and mobility activation energy (E_μ) were investigated by the TW method.

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The concept of the TW method is explained as follows. There is a surface acoustic wave (SAW) excited by a transducer on the surface of the $LiNbO_3$ crystal. Owing to the piezoelectric properties of the $LiNbO_3$ crystal, a travelling electromagnetic wave produced by the SAW couples into the films. A dc acoustic-electric current (I_{ae}) or voltage (V_{ae}) can be obtained. Thus σ_d and μ_d can from be calculated from I_{ae} or V_{ae}, which can be found from our earlier paper.[5] The activation energies E_σ and E_μ can thus be calculated from the temperature dependence of σ_d and μ_d in the range of 300 to 450K.

Ⅲ. RESULTS AND DISCUSSION

The typical XRD pattern of the sample with a hydrogen dilution ratio of 0.33% is shown in Fig.1. There are three diffraction peaks corresponding to the (111), (220) and (311) planes. This demonstrates that the series of the samples are crystallized. An average grain size is estimated to be about 20 nm from the full width at half maximum (FWHM) of the peaks by the Scherrer formula for ⟨111⟩ orientation.

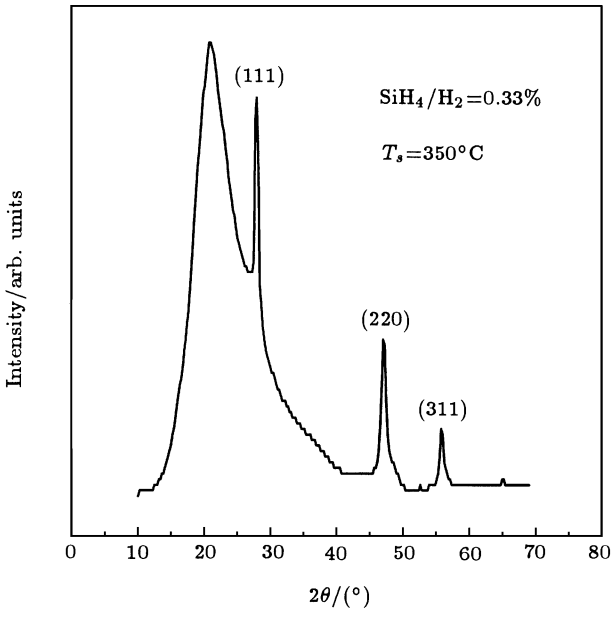


Fig.1. A typical XRD pattern of the μc-Si:H film with hydrogen dilution R=0.33%.

Figure 2 shows the typical micro-Raman spectrum of the sample with a hydrogen dilution ratio of 0.33%. A peak located at 516.3cm^{-1} can clearly be seen, which reveals that the sample has been crystallized. In order to estimate f_c in the sample, we use the 520cm^{-1} peak corresponding to the phonon vibration mode of crystalline silicon, the 500cm^{-1} peak corresponding to silicon of wurtzite structure, and the 480cm^{-1} peak corresponding to amorphous silicon to analyse the integrated area ratio of the 516.3cm^{-1} peak.[6] The result is that f_c varies monotonically from 73% to 76% with decreasing R from 2% to 0.2%.

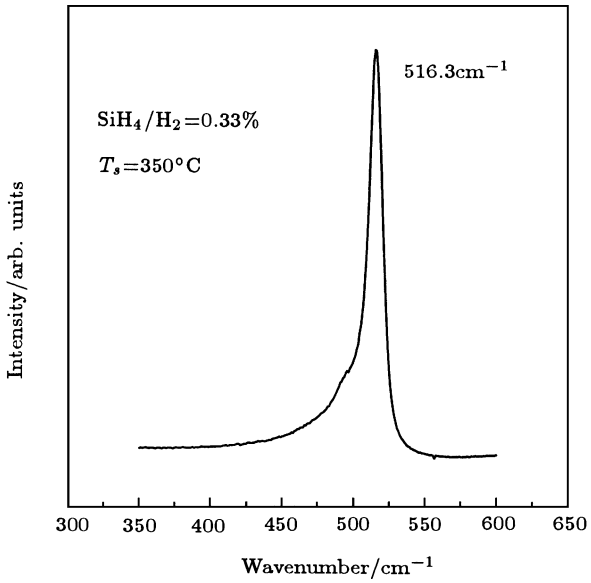


Fig.2. A typical Raman spectrum of the μc-Si:H film with hydrogen dilution R=0.33%.

The room-temperature drift mobility (μ_d) and its activation energy (E_μ) versus R is shown in Fig.3. With decreasing R from 2% to 0.2%, μ_d increases from 8.9×10^{-3} to 5.5×10^{-1}cm^2/Vs and E_μ decreases from 129 to 82meV.

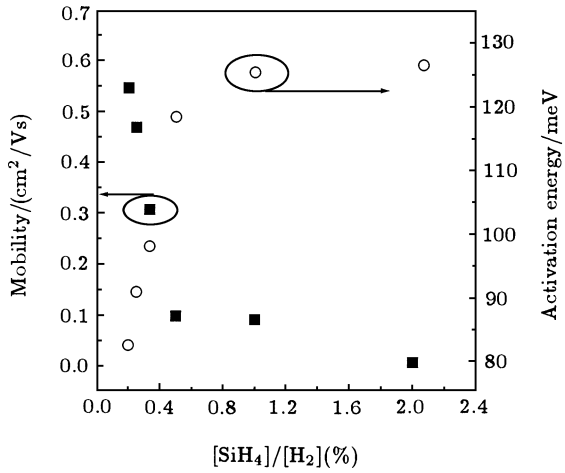


Fig.3. The dependence of room-temperature drift mobility and its activation energy on different hydrogen dilution ratios.

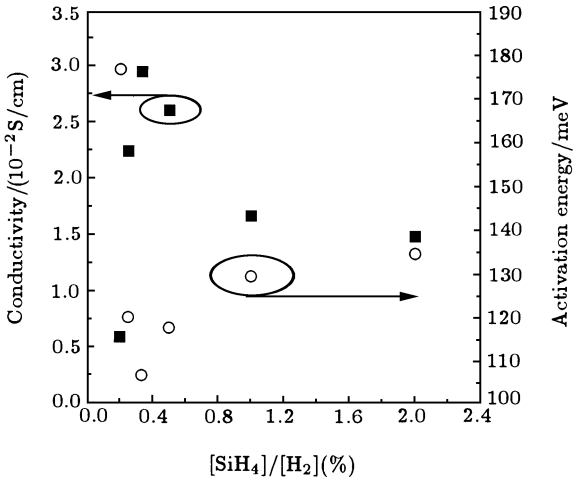


Fig.4. Room-temperature dark conductivity and its activation energy as a function of different hydrogen dilution ratios.

Figure 4 shows the room-temperature dark conductivity ($\sigma_{\rm d}$) and its activation energy (E_σ) as a function of R. The $\sigma_{\rm d}$ increases from 1.5×10^{-2} to 2.9×10^{-2}S/cm and E_σ decreases from 134 to 106meV with R from 2% to 0.33%. When R continuously decreases to 0.2%, $\sigma_{\rm d}$ decreases to 5.9×10^{-3}S/cm and E_σ increases to 176meV.

From the XRD and Raman scattering results, the mixture of crystalline and amorphous phases was observed in our μc-Si:H films. Therefore, the grain-boundary potential barrier scattering model could be adopted to explain the transport properties. In our μc-Si:H films, most defects are located at the boundaries of the crystallites.[7] Carriers trapped in grain-boundary defects give rise to potential barriers. These barriers limit the carrier transport between crystallites and thus dominate the transport properties of the films.[8]

According to the results of microstructures, the average grain size is almost unchanged and the crystalline volume fraction increases when R decreases. So the widths of the potential barriers become thinner with decreasing R. Hydrogen dilution helps to reduce the defect density in μc-Si:H films. When R decreases, the decrease of the defect density lowers the height of the potential barriers and reduces the scattering effect of carriers. So $\mu_{\rm d}$ is increased with decreasing R.

Another effect of hydrogen dilution during deposition is the hydrogen plasma etching,[4] which will effectively remove the weak bands from the films, and improve the local order of the amorphous phase. So, with decreasing R, both band tails and the density of localized states in the band tails will be reduced, and consequently the density of intrinsic carriers decreases. In μc-Si:H films, the density of carriers and the drift mobility mainly determine the dark conductivity. With decreasing R, the drift mobility is increased, while the density of carriers decreases. Therefore, the dark conductivity exhibits a maximum value of 2.9×10^{-2}S/cm at the hydrogen dilution of 0.33%. These properties are different from those of traditional μc-Si:H films prepared with hydrogen-diluted silane plasma.

IV. CONCLUSIONS

In summary, highly hydrogen-diluted silane plasma has been employed to deposit a series of undoped μc-Si:H films in a PECVD system with various hydrogen dilution ratios. It was found that the samples are mixtures of crystalline and amorphous phases. The mean size of the crystalline grains is around 20nm and the crystalline volume fraction in the μc-Si:H films is about 75% for different hydrogen dilution ratios R. For the transport properties of the samples, the drift mobility increases from 8.9×10^{-3} to 5.5×10^{-1}cm^2/Vs, and the dark conductivity first increases from 1.5×10^{-2} to 2.9×10^{-2}S/cm and then decreases to 5.9×10^{-3}S/cm when R decreases from 2% to 0.2%. The grain-boundary potential barrier scattering model is adopted to explain the transport mechanism.

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