Structural and Chemical Features of Si Nanocrystallites in nc-Si:H Films

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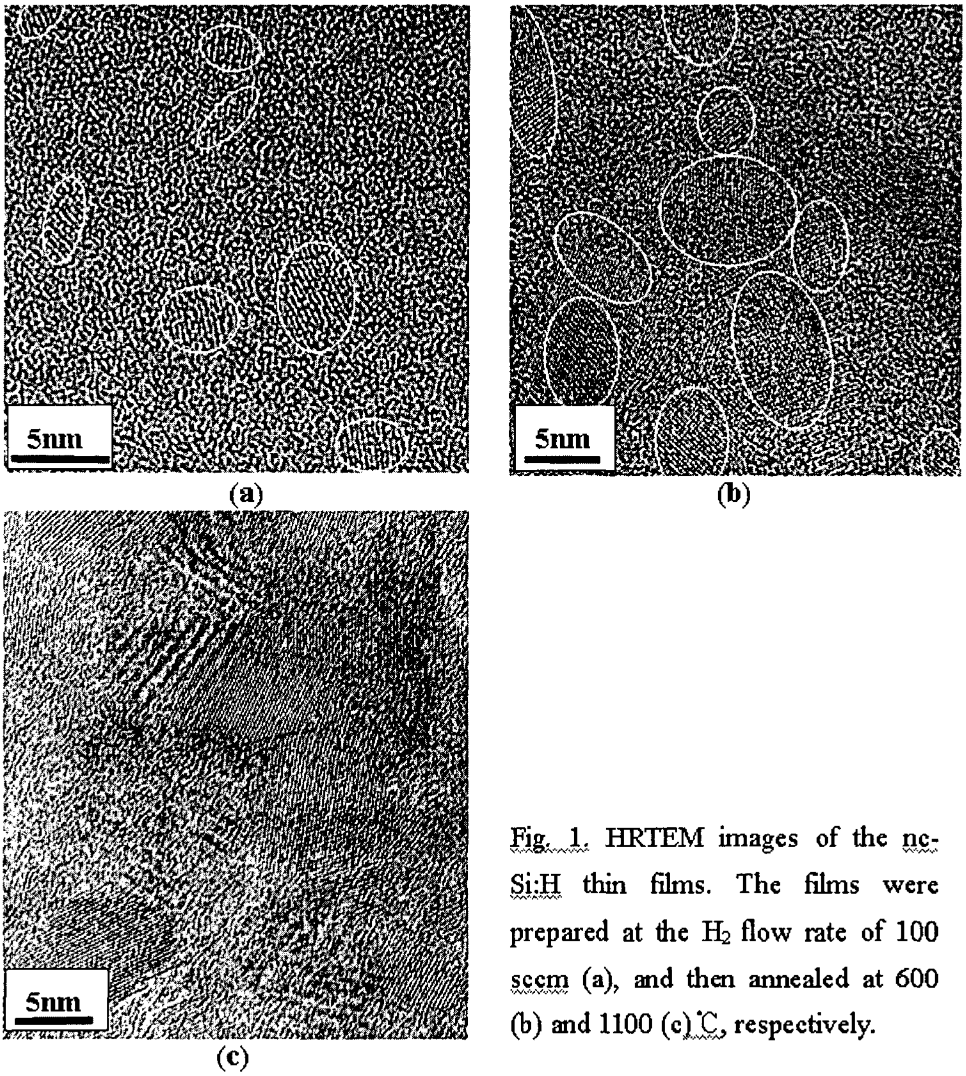
Nanocrystalline hydrogenated silicon (nc-Si:H) thin films have attracted much attention due to their potentialapplication in various devices. In particular, it is expected that these materials can be used to fabricate micro- and opto-electronic devices compatible with Si integrated circuit technology. Recently, it has been known that quantum size effects of Si nanocrystallites are the main source for the unique and useful optical features of the nc-Si:H thin films.

In this study, we investigatedthe hydrogen effects on the nanostuctural features of nc-Si:H thin films, based on the structural and chemical analysis; the films were prepared by plasma enhanced chemical vapor deposition (PECVD) techniques. The nanostructural and chemical features of nc-Si:H thin films were investigated as a function of deposition conditions. SiH_4 gasflow rate was varied to control the amount as well as the type of hydrogen-related bonds in the films.

It was found that the crystallite size varied with the relative fraction of $Si\text{-}H_3$ bonds in the films, n=integer, which was sensitively related with the flow rate of $[Si-H_3]/\sum_{n=1}^{3}[Si-H_n]$ SiH_4reaction gas. The Si nanocrystallites in the films enlarged from ~2.0 to ~8.0 nm in their size with increasing the SiH_4gas flow rate from 8 to 20 sccm, while the PL emission energy varied from 2.5 to 1.8 eV; the relative fractions of the $Si\text{-}H_3$, $Si\text{-}H_2$, and Si-H bonds in the amorphous matrix were also varied sensitively with the SiH_4 gas flow rate. A model for the nanostructure of the nc-Si:H films was suggested to feature the variation in the size and chemical bonds of the nanocrystallites as well as the amorphous matrix depending on the deposition conditions.

Fig. 1 shows HRTEM images of as-prepared nc-Si:H thin films (a), and the samples post-deposition annealed at 600 (b) and 1100 ℃(c), respectively. These micrographs illustrate the presence of about 4.0 ~ 10.0 nm-sized Si nanocrystallites in the films. In particular, the size of the nanocrystallites in the as-prepared films ranges from ~ 2 to ~ 4 nm. It is clearly seen that the nanocrystallite size increases after the post-deposition annealing at 400 ~ 1100 ℃ isolated nanocrystallites are dispersed in the amorphous matrix of the as-prepared films and the samples post-deposition annealed at 600 ℃. However, the crystallites appear to be joined each other and overlapped in the samples post-deposition annealed at 1100 ℃.



(a)

(b)

(c)

Fig. 1. HRTEM images of the nc-Si:H thin films. The films were prepared at the H_2 flow rate of 100 sccm (a), and then annealed at 600 (b) and 1100 (c) ℃, respectively.