Formation of nanocrystalline silicon thin-films through magnesiothermic reduction of quartz-substrates

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Introduction: Silicon (Si) is the most abundant semiconductor-material found in form of silica (SiO_2) that contributes to the large-scale to microelectronics, and optoelectronics-field *etc*. In particular, nanocrystalline Si (nc-Si) is promising for future optoelectronics, since it shows material properties which combine advantages of both amorphous-Si and polycrystalline-Si. However, current methods of obtaining nc-Si thin-films involve re-crystallization of amorphous-Si, or direct deposition of nc-Si through plasma enhanced chemical vapor deposition (CVD), hot wire CVD, glow discharge CVD *etc*. Various complex-steps, requirement of higher process-temperature, and application of toxic materials in the above techniques limit its potential applications.

We propose a simple method for the formation nc-Si thin-films on low cost substrate (silica: glass or quartz *etc*) through metallothermic reduction. Particularly, in this study, we have focused on the formation of nc-Si-film through magnesiothermic reduction of quartz (SiO_2). According to thermodynamic properties of SiO_2, magnesiothermic reduction occurs around melting temperature of magnesium (Mg), which is around 650° C following the basic equations:

$$SiO_2\ (Solid) + 4e^- \rightarrow Si\ (reduced) + 2O^{2-} \quad (1)$$
$$Mg\ (s) \rightarrow Mg^{+2} + 2e^- \quad (2)$$
$$SiO_2\ (s) + 2Mg \rightarrow 2Si\ (s) + 2MgO \quad (3)$$

Experimental: Mg thin-films with thickness of ~ 1 μm were deposited through RF magnetron sputtering on quartz-substrates. Then, Mg/quartz structure was transferred to a thermal annealing system, where it was annealed at 700° C in the vacuum; thereby, going through a magnesiothermic reduction, where surface of the quartz-substrate reduced to become Si-film. Several samples were prepared by changing the annealing time ranging from 1 ~ 9 hours. Obtained Si-films were characterized by Raman spectroscopy, photoluminescence, scanning electron microscopy (SEM), and optical absorbance measurement *etc*.

Results and Discussions:

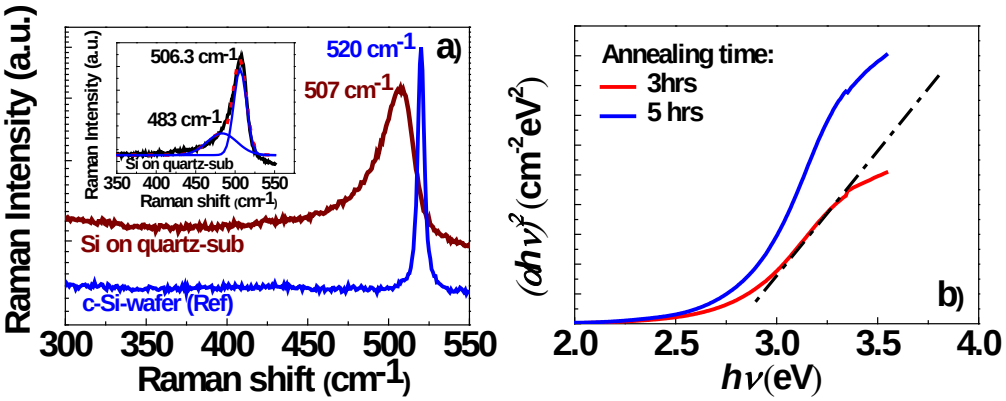

Fig.1 (a) Raman spectra of magnesiothermic reduced Si-film on quartz-substrate. Inset of the figure shows fitting of the Raman spectrum; (b) Band-gap determination from data obtained by UV-visible measurement.

Shown in Fig. 1(a) is the Raman spectroscopy of the Si-thin film on the quartz-substrate, obtained through magnesiothermic reduction at 700° C with 3-hours of reaction time. Raman spectrum of the oriented single crystal Si-wafer has been shown as a reference. An asymmetric peak at ~507 cm^{-1} has been apparent for the Si-film on the quartz-substrate. Fitting of the Raman spectra (inset of the figure) shows Gaussian-deconvolution of the two peaks centered around ~ 480 cm^{-1}, and 506 cm^{-1}, respectively. Peak at 506 cm^{-1} roughly suggests formation of nc-Si with evolution of small amorphous phase at 480cm^{-1}. Optical band-gap (E_g), of the Si-film obtained by absorption measurement was found around 2.8 eV, which is characteristic for the nc-Si thin-films. Annealing time was varied during reduction to study the effect of reaction time on the quality of the nc-Si film. Optical and structural properties were discussed in relation to the various annealing time at 700°C.