Hydrogen-Induced Defects in Poly-Si Thin Films Observed by Raman Spectroscopy

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Polycrystalline Silicon (poly-Si) for thin-film transistor (TFT) has been fabricated by various techniques such as solid-phase crystallization (SPC), excimer-laser annealing (ELA) and continuous-wave laser lateral crystallization (CLC).¹ It is known that hydrogenation significantly improve performance of TFT due to the termination of dangling bonds (DBs) at defects. Although intentional hydrogenation is not always required for current poly-Si films, exposure to atomic hydrogen is still essential to TFT process. It should be noted that hydrogen not only improves TFT performance but also generates excess defects in films.²

We have investigated local-vibration modes (LVMs) of Si-H bonds in poly-Si films using Raman spectroscopy. ^{3,4} Two dominant bond-stretching modes were observed at 2000 and 2100 cm⁻¹, where the observed bands depend on crystallization techniques and hydrogenation conditions. The 2000 cm⁻¹ band was attributed to DB's at grain boundaries and the 2100 cm⁻¹ band was to ingrain defects generated by both rapid cooling after laser irradiation and exposure to atomic hydrogen. In this paper, we report on the interaction between defects and hydrogen investigated by excess hydrogenation for poly-Si.

Used samples are mainly ELA poly-Si films crystallized with three different energy density, E_L , of 200, 230 and 260 mJ/cm², where the average grain sizes are 0.10, 0.18, and 0.58 μ m, respectively. Poly-Si films crystallized by SPC and CLC and single crystalline Si(100) bulk were also examined. Hydrogenation was performed for time, t_H , of 1-90 min using remote plasma enhanced by 2.45 GHz microwave, where plasma was transferred to poly-Si films maintained at 350°C in down stream without electric acceleration. For plasma-free hydrogenation, catalytic method using a tungsten hot wire was also used.¹

Typical LVM spectra for a device-graded a-Si:H film and hydrogenated poly-Si films are shown in Fig. 1. As well as for a-Si:H, the 2000 cm⁻¹ band was observed for all poly-Si films besides CLC. On the contrary, the 2100 cm⁻¹ band was found only for ELA-poly-Si. The intensity of 2000 and 2100 cm⁻¹ bands, I_{2000} and I_{2100} , for ELApoly-Si are plotted as a function of t_H in Fig. 2(a) and 2(b), respectively. I_{2000} decreases with increasing E_L and is almost constant for varying t_H , that is the intensity saturates for t_H so short as 1 min. Those variations are interpreted by the assignment of 2000 cm⁻¹ band to DBs at grain boundaries. The variation of I_{2100} depends on E_L . For $E_L = 200 \text{ mJ/cm}^2$, I_{2100} is almost constant for varying t_H . For E_L =230 and 260 mJ/cm², I_{2100} increase with increasing t_{H} . Those variations indicate that 2100 cm⁻¹related defects are generated during hydrogenation. That is, incident hydrogen atoms break deformed Si-Si bonds (weak bonds) neighboring to defects leading to termination with 2100 cm⁻¹-related Si-H bonds. Thus it is deduced that the larger the defect density in original films, the larger the 2100 cm⁻¹ LVM intensity. In practice, the 2100 cm⁻¹ band was not found for single crystalline

Si(100) hydrogenated under the present conditions. Moreover, no LVM was found for CLC poly-Si films as shown in Fig. 1, which indicates that the defect density in CLC poly-Si is apparently smaller than in ELA. The weak bond model has been previously mentioned not only as a term of hydrogen but also ultra-violet (UV) light irradiation.⁵ The effect of UV light on generation of the 2100 cm⁻¹ LVM is now under the progress.

In conclusion, it was shown that exposure of poly-Si films to atomic hydrogen not only terminates DBs at grain boundaries but also generates defects in grains. That effect is especially obvious for films with large defect density.

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Fig. 1 LVM spectra observed for an a-Si:H film and hydrogenated poly-Si films crystallized by SPC, ELA and CLC techniques. Hydrogenation was performed

by catalytic method.



Fig. 2 Relationship between hydrogenation time and LVM intensity for ELA poly-Si crystallized with three different energy densities.