Area: Area 1 Crystalline and Thin Film Silicon PV

INFLUENCE OF NON-BONDED HYDROGENS ON AMORPHOUS SILICON NETWORK IN HYDROGENATED AMORPHOUS SILICON

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Hydrogenated amorphous silicon (a-Si:H) with low defect density has been applied in thin-film transistor and solar cells. The low defect density can be achieved by the hydrogen termination of dangling bonds in a-Si network, resulting in Si-H_x bonds within vacancies and voids. Not only the bonded hydrogens (BHs) but non-bonded hydrogens (NBHs), most likely H_2 molecules, can be contained in the a-Si network. Hydrogenated amorphous germanium (a-Ge:H) with high NBH content (C_{NBH}) up to about 12 at.% was reported, and it was suggested that NBHs in interstitial or inside small voids apply compressive stress on void-walls [1]. However, it was not clear the influence of NBHs on the a-Si network.

For this issue, recently, we have reported that the presence of large amounts (2.8-3.9 at.%) of NBHs in a-Si:H resulted in broadening of the vacancy size (N_V) distribution [2]. The N_V was calculated from the empirical equation of $N_V = -4.6(\tau - 0.218)/(\tau - 0.484)$ [3], where τ is the positron lifetime determined using positron annihilation lifetime spectroscopy. $C_{NBH} = C_T - C_{LSM} - C_{HSM}$, where total hydrogen content (C_T) and bonded hydrogen content (C_{BH}) were quantitatively determined by Rutherford backscattering spectroscopy (RBS)/ hydrogen forward scattering and Fourier transform infrared spectroscopy, respectively. $C_{BH} = C_{LSM} + C_{HSM}$, where C_{LSM} and C_{HSM} are bonded hydrogen contents contributing to low (~2000 cm^{-1}) and high stretching modes (~2100 cm^{-1}), respectively.

In Figure 1, we showed the positron annihilation lifetime distribution for crystalline silicon (c-Si) and three types of a-Si:H films (standard, high C_{HSM}, and high C_{NBH}) deposited using plasma-enhanced chemical vapor deposition on glass substrates. All a-Si:H films mainly contained divacancies with $N_V = 2$, but nanovoids with $N_V \geq 5$ existed in the film with high C_{HSM}. The size of the nanovoids with $N_V = 5$ and 6 was ~1 nm [3]. Interestingly, for the film with high C_{NBH}, $N_V < 1$ and $N_V \geq 5$ were shown simultaneously. The a-Si network will become unstable when the C_{NBH} exceeds the solubility limit of NBH (C_{SLNBH}). We estimated that $1.5 < C_{SLNBH} \leq 2.8$ (at.%). RBS data showed that the atomic number density of the silicon (N_{Si}) for the high-C_{NBH} film (4.88×10^{22} cm^{-3}) was larger than the standard film ($4.83\text{-}4.86 \times 10^{22}$ cm^{-3}) and the high-C_{HSM} film (4.05×10^{22} cm^{-3}). Moreover, we revealed the contribution of the NBHs to the optical bandgap (E_{opt}) from transmittance and reflectance measurements: $E_{opt} = 2.16C_{LSM} + 1.09C_{HSM} + 1.18C_{NBH} + 1.40$ (eV). This meant that NBHs in addition to BHs maintain the compressive stress in the a-Si network, similar to the case of a-Ge:H [1].

In summary, NBHs in small vacancies induced large nanovoids (> ~1 nm), via the stress relaxation due to the creation of nanovoids, without decreasing the N_{Si} as shown in Figure 2. The above-mentioned data and the further investigation of the influence of NBHs on the a-Si network will be discussed.

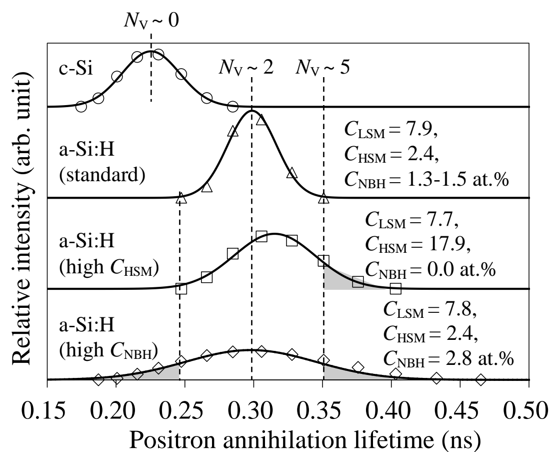

Figure 1: Positron lifetime distribution in terms of relative intensity vs lifetime.

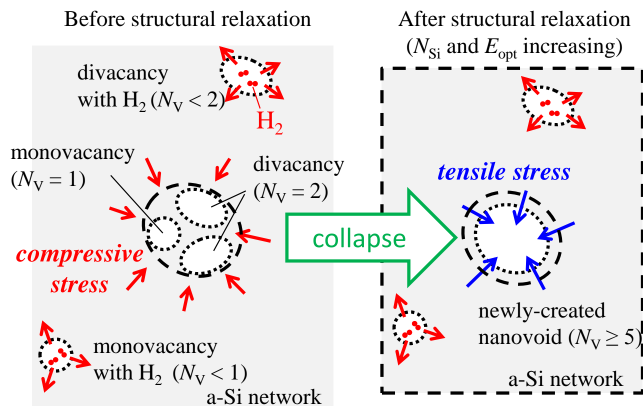

Figure 2: Schematic representation of NBH-induced structural change.

[1] F.C. Marques et al., J. Appl. Phys. 84 (1998) 3118.
[2] T. Sekimoto et al., J. Non-Cryst. Solids 447 (2016) 207.
[3] G. Amarendra et al., Phys. Rev. B 63 (2001) 224112.