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Novel insights into the structural and electrical properties of metastable defects in hydrogenated amorphous silicon

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ABSTRACT

Due to the complex nature of the hydrogenated amorphous silicon (a-Si:H) nanostructure there is a limited understanding of the native and metastable defects and recombination in this material. This has proven to be a major obstacle in finding the origin of the Staebler-Wronski effect (SWE) [1]. The limited understanding of the nanostructure and defect states has led to a wide variety of models [2-4] that try to describe the SWE, none of which have yet succeeded in providing convincing experimental evidence for their correctness. On the road towards SWE reduction we therefore present the latest insights into the structural and electrical properties of metastable defects in a-Si:H using continuous wave electron-paramagnetic resonance (cw-EPR) spectroscopy, time-domain pulsed EPR spectroscopy [5] and Doppler broadening positron annihilation spectroscopy (DB-PAS) [6,7].

The spin density of various a-Si:H materials with varying nanostructures is determined through cw-EPR spectroscopy. The observed correlation between the spin density and the Doppler S parameter, as obtained through DB-PAS, indicates that porous materials that are dominated by larger open volume deficiencies exhibit higher spin densities, while dense materials that are dominated by smaller open volume deficiencies show smaller spin densities. However, after light soaking more similar spin densities are observed, indicating a long term defect creation process in the SWE that is less dependent on the a-Si:H nanostructure when compared to the initial state.

Large differences are observed for the various a-Si:H nanostructures in the echo decay obtained from time-domain pulsed EPR spectroscopy. It appears that a superposition of two exponentially decaying functions with different phase memory relaxation time constants $T_{m1,m2}$ and EPR spectral amplitudes $A_{1,2}$ can be used to accurately fit the normalised ESE decays, as has recently been demonstrated [5]. This means that the SWE can be described in terms of a fast relaxing type I defect (T_{m1} = 1.2 µs) and a slow relaxing type II defect (T_{m2} = 10±2 µs). Both A_1 and A_2 increase after light soaking, but the relative increase is generally larger for A_2, especially for dense a-Si:H material that shows a low Doppler S parameter. Since such dense a-Si:H is known to exhibit a good light soaking stability, it appears that the SWE is limited by isotropically distributed defects in high quality samples. This suggests that type II defects are linked to open volumes (non-clustered spins) while type I defects correspond to smaller volume deficiencies, such as divacancies (clustered spins). A high initial value of the A_1/A_2 ratio seems to be linked to improved stability, which suggests that reducing the nanosized void density while increasing the hydrogen passivation degree of small open volume deficiencies as much as possible is the recipe for making the most stable a-Si:H. Such an enhanced understanding of the complexity of the light-induced defect formation kinetics can prove to be a useful tool in understanding the nature of metastable defects in a-Si:H and reducing the SWE in the production process of a-Si:H based solar cells.

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#	p [mbar]	P_{rf} [W/cm^2]	Φ_{H2} [sccm]	Φ_{SiH4} [sccm]	r_d [nm/min]	T_{sub} [°C]
dense R=0	0.7	0.024	0	40	11.1	180
dense R=10	2	0.024	200	20	6.25	180
porous R=0	1	0.069	0	40	43.0	160
high p R=50	8	0.069	200	4	11.0	150

Table 1: Deposition conditions for a-Si:H films with varying nanostructures.

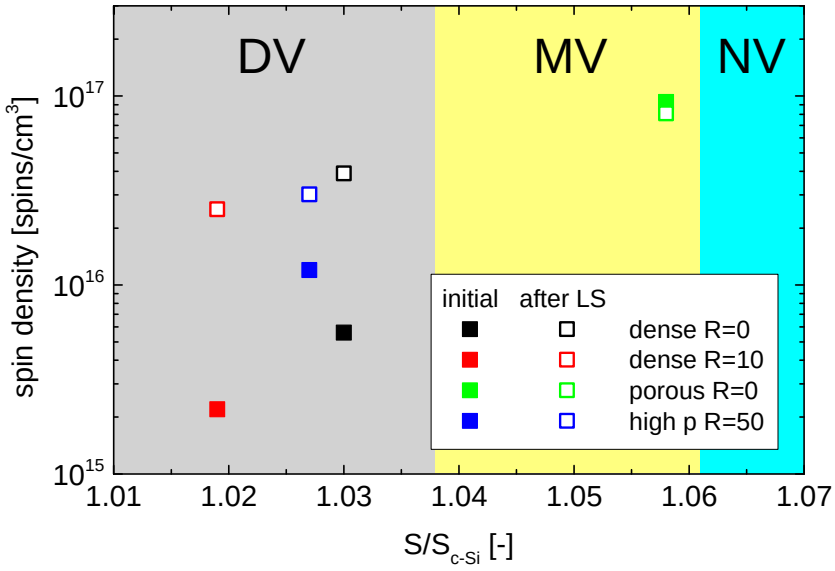

Figure 1: Correlation between Doppler S parameter (normalised to the Doppler S parameter of crystalline silicon) and spin density for different a-Si:H materials both in the as deposited state (initial) and light soaked state (after LS). For different values of $S/S_{c\text{-}Si}$ the dominant type of open volume deficiency in the material can be either divacancies (DV), multivacancies (MV) or nanosized voids (NV).

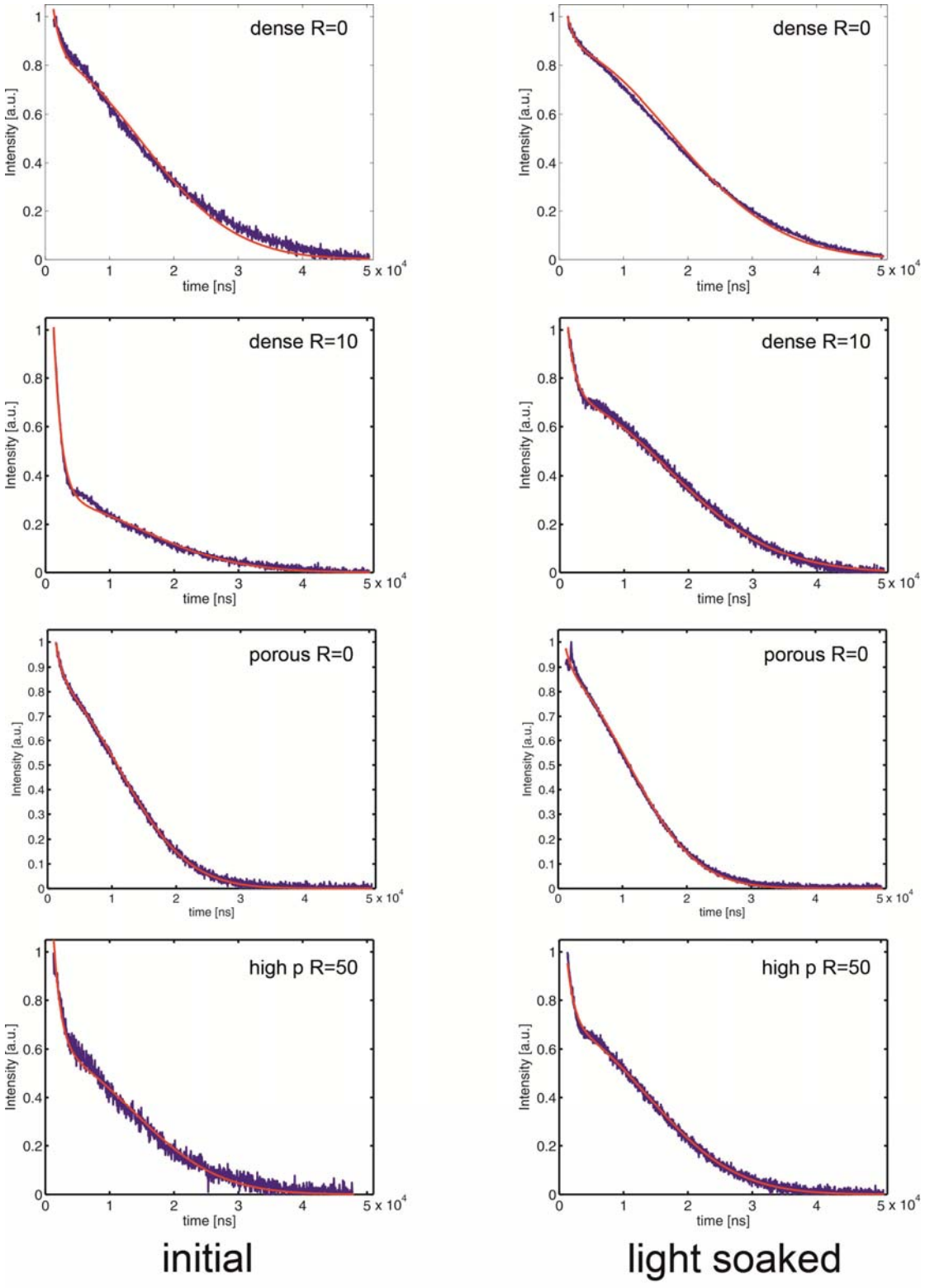

Figure 2. Normalised ESE decays of various a-Si:H materials (blue) and fitted stretched-exponential functions (red) both in the initial state (left) and light soaked state (right). All spectra were recorded at the same microwave frequency.

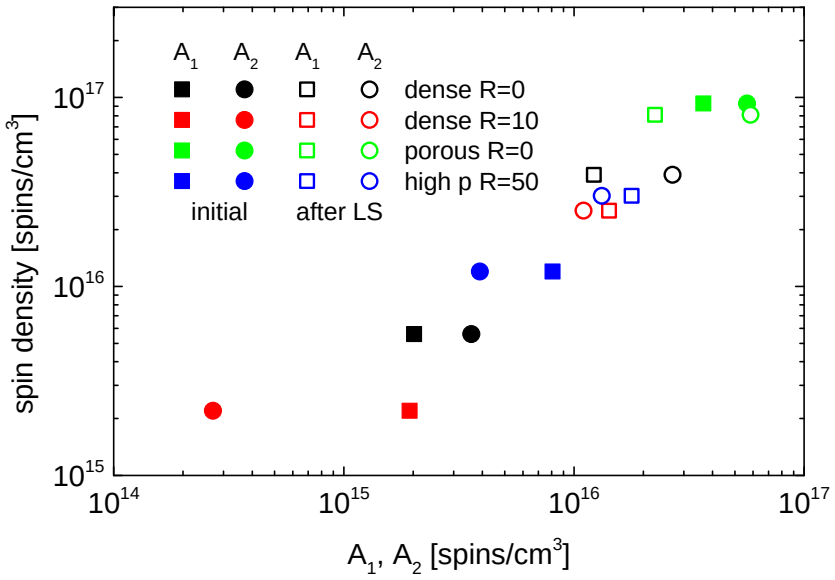

Figure 3: Correlation between A_1 and A_2 and the total spin density for various a-Si:H materials with varying nanostructure both in the initial state (closed symbols) and the light soaked state (open symbols).

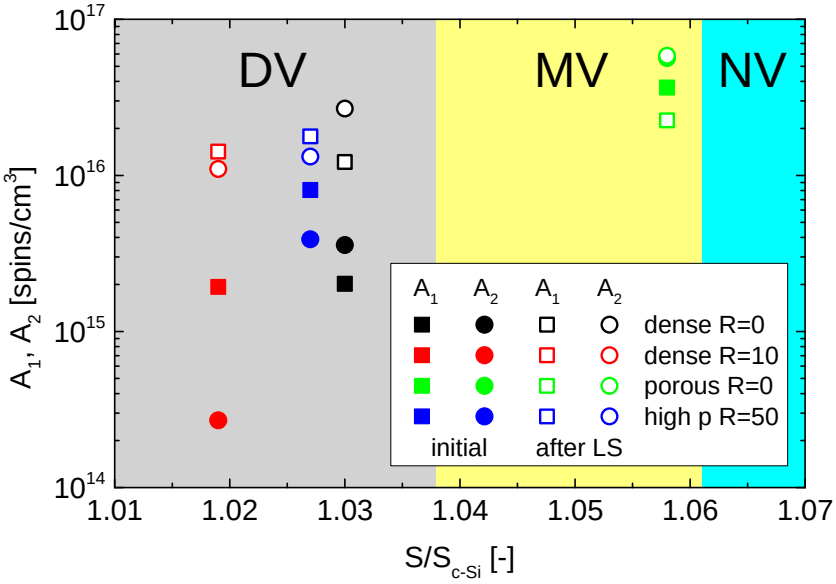

Figure 4: Correlation between Doppler S parameter and A_1 and A_2 for various a-Si:H materials with varying nanostructures both in the initial state (closed symbols) and the light soaked state (open symbols). For different values of $S/S_{c\text{-}Si}$ the dominant type of open volume deficiency in the material can be either divacancies (DV), multivacancies (MV) or nanosized voids (NV).