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Voids and molecuar hydrogen in hydrogenated amorphous silicon RAJENDRA TIMILSINA, PARTHAPRATIM BISWAS, The University of Southern Mississippi — Nuclear magnetic resonance (NMR) and Infrared (IR) spectroscopy experiments show that hydrogen microstructure consists of clustered and diluted hydrogen atoms as well as voids and hydrogen molecules in hydrogenated amorphous silicon. Several theoretical studies have also attempted that whether the microstructure incorporates voids and hydrogen molecules or not, by introducing hydrogen atoms within artificially created cavities, after relaxing the models of hydrogenated amorphous silicon. However, no theoretical study, up until now, has conclusively demonstrated that the voids and molecular hydrogen are built-in features of the microstructure. We generate several realistic models of hydrogenated amorphous silicon at different hydrogen concentrations by developing an information-based inverse method. The models not only satisfy structural and electronic properties but also provide correct NMR line spectra as compare to NMR experiments. The microstructure at high (>15%) hydrogen concentration shows the presence of voids and some hydrogen molecules within the voids. The voids with molecular hydrogen are built-in configurations of the microstructure because they evolve themselves while relaxing the models via the first-principles density functional method.

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