Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

The role of hydrogen on the structural properties of nanocrystalline silicon ALESSANDRO MATTONI, CNR-IOM Cagliari — Hydrogenated nanocrystalline silicon (nc-Si:H) is an emerging thin-film photovoltaic material that combines advantages of silicon (c-Si), like high carrier mobility, with less expensive production methods of amorphous silicon (a-Si). Among several processing issues, hydrogenation is critically in affecting the structural and electronic properties of nc-Si[1]. Here, we report molecular dynamics theoretical results on the effect of dissolved hydrogen on the thermally induced recrystallization[2] of nanocrystalline silicon. The recrystallization rate decreases exponentially with hydrogenation with a tendency of H atoms to out-diffuse to the crystal phase at low concentration and forming immobile SimHn hydrides at higher concentration[3]. The tendency of H to segregate in the amorphous enables quantum confinement phenomena with the holes localized within the crystal grains. The possibility to tune the electronic gap of the material by the grains size is showed by semi-empirical and ab initio electronic structure calculations on large scale atomistic models[4].[1] L. Bagolini et al. PRL 104, 176803 (2010);[2] A. Mattoni et al., PRL 99, 205501 (2007); 78 075408 (2008); [3] G. Fugallo and A. Mattoni, submitt (2013); [4] A. Mattoni et al., 79, 245302 (2009);

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Date submitted: 16 Nov 2013 Electronic form version 1.4