Photovoltaic effect with a high open circuit voltage \( (V_{oc}) \) has been observed in thin free standing pn type layer of electrochemically prepared nanocrystalline silicon material (nc-PSi), indicating the possibility that the material acts as a wide gap material [1]. The conversion efficiency and stability of the material are strongly limited by the material high resistivity partially due to the presence of a high density of surface states and by the intrinsic instability of that large hydrogen passivated internal surface. Consequently, new passivation techniques are currently under investigation to improve the performance and stability of the material. In this study, three different types of modification were investigated: surface chemical modification (SCM) by organic molecules (alkene, aldehyde, carboxylic groups, etc…) [2], electrochemical oxidation (ECO) in \( \text{H}_2\text{SO}_4 \), as well as monomer polymerization (pyrrole) in the silicon material matrix.

The typical photovoltaic and spectral responses of pn type nc-PSi devices before and after various passivation treatments are shown in Fig. 1. As prepared material is characterized by a \( V_{oc} \) up to 0.875V, a limited shortcut current density \( (J_{sc}) \) and a spectral response with a peak located at 450 nm. As observed in Fig. 2, the range of recorded PV characteristics \( (V_{oc} \text{ and } J_{sc} \text{ over several devices}) \) shows strong inter-sample variations [3], probably due to uncontrolled parameters during the formation of the material. After modification through SCM, a strong increase in current has been observed with aldehyde molecules (decanal, Si-O-C bonding) but not with alkene or carboxylic group species (Si-C bonding). A similar but limited increase in photocurrent was also observed after ECO treatment with almost no modification of the photovoltage or PV characteristics spread. Oppositely, samples that were filled with poly-pyrrole showed a strong reduction of the characteristics spread with an average increase of the resulting open circuit voltage. A decrease of the photogenerated current was also observed due to light absorption in the outer poly-pyrrole layer. Oxidation of the silicon surface is also expected to occur during polymerization of the pyrrole monomer. Beside pyrrole, polymerization of aniline monomer in nc-Psi is under investigation as well due to its higher transparency in the visible spectrum. The previous results clearly show the strong involvement of the surface condition on the observed PV effect and the necessity to get a deeper understanding of the photoconduction phenomena in the material.

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