Surface and composition bandgap engineered Si based nanocrystals in solar cells

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Motivation

- Novel concepts ⟹ innovative approaches to material synthesis are essential to enhance significantly solar cell performance
- Silicon ⟹ compatibility with cutting-edge photovoltaic technologies and natural environmental
- Carrier multiplication in silicon nanocrystals (Si-ncs) (A. Nozik) NanoLett. 7 2506 (2007) D. Timmerman et al. *Nat. Photonics* **2008**, 21, 105. D. Timmerman et al. *Nature Nanotechnology*; 2011 6, 710
- Not yet demonstration in solar cell

Problems ⟹ Si energy band gap at quantum confinement probably too wide
Surface play signuificant role at quantum confinement

Approaches ⟹ Nanocrystals surfactant free 3D surface engineering at quantum confinement effects
Si alloying with tin (Sn) might opens opportunity to decrease the band gap

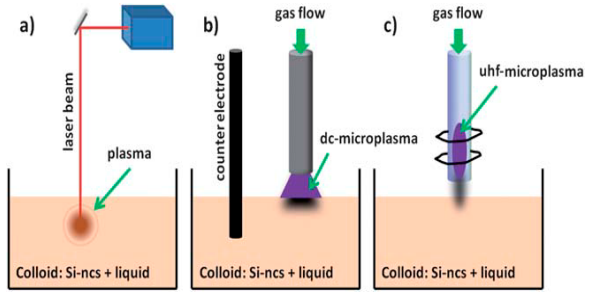
Nanocrystals 3D surface engineering

- Surface engineering without surfactant at quantum confinement size (< 5 nm)
- Microplasma induced chemistry

ns/fs laser generated plasmas under colloid (Si-ncs in water/ethanol) surface

DC microplasma generated between Ni tubing & colloid (He 250 SCCM))

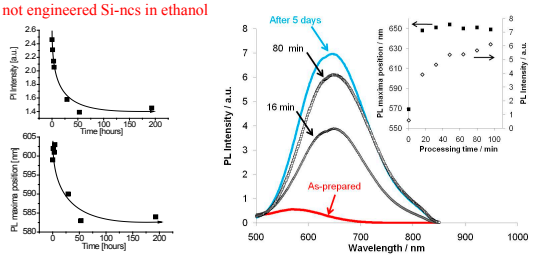
Plasma generated between RF & ground electrode (60W@450MHz) (He 250 SCCM)

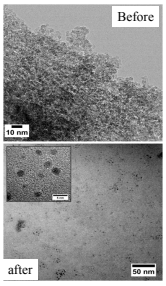


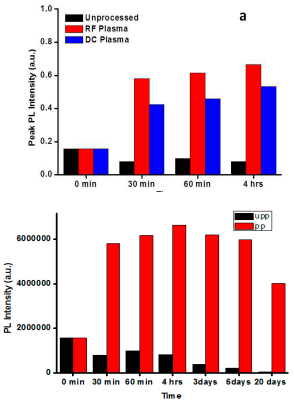
- 3D surface engineering of Si-ncs in aqueous is the most efficient in case of RF microplasma

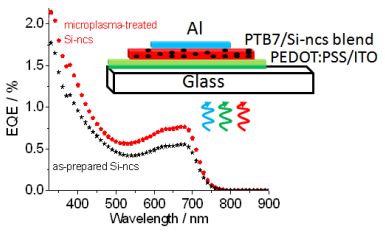
- Increased PL intensity and stability from Si-ncs

not engineered Si-ncs in ethanol







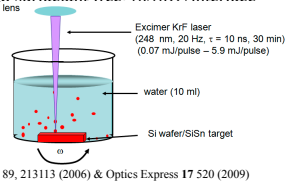


- Electrons impact at Si-ncs surface and replace the H-terminations located on the surface of Si-ncs
- Hybrid solar cells performance improvement after Si-ncs engineering

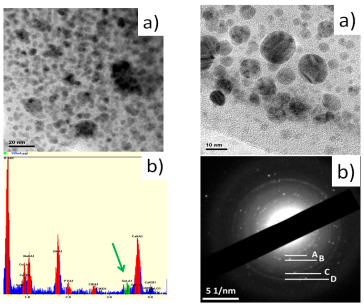
Svrcek et al. J. of Phys. Chem. C **115**, 5084 (2011). Appl. Phys. Lett. 97 161502 (2010) Adv Function Mat, 22 954 (2012) , Nanoscale 5 (4), 1385 (2013), Svrcek et al APL 100 223904 (2012)

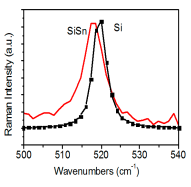
Energy band gap engineering

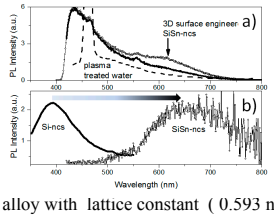
- Confined plasma in liquid medium (7GPa)
- Cloud of Si/Sn atoms and embryotic particles in liquid G=G(P)
- Water and surfactant free Si/SiO$_x$ interface



Svrcek et al. APL, 89, 213113 (2006) & Optics Express **17** 520 (2009)







- SiSn-ncs in cubic crystalline alloy with lattice constant (0.593 nm) between the bulk values Si and Sn of 0.543 nm and 0.649 nm)
- Increased PL after 3D surface engineering (red-shifted by more than 250 nm compared to PL peak emission of typical elemental Si-ncs.

Conclusions

- RF microplasma compared to DC more efficient stabilization for the Si-ncs in water
- Engineering of surface/interface with polymers enhanced efficiency of hybrid solar cells
- Confined laser plasma in water allowed the growth of alloyed semiconducting silicon tin nanocrystals (SiSn-ncs)
- Both alloying and nano-stracturing challenge the Si indirect nature

ACKNOWLEDGMENTS This work was also partially supported by a NEDO project and JSPS invitation and JSPS Bridge fellowships