Mesoscale modeling of quantum yield in nanocrystalline devices

A new solar material features silicon nanocrystals (nc-Si) within an amorphous silicon (a-Si) matrix. The efficiency with which photons are absorbed and converted to electric current depends on the size, orientation, volume fraction, and interface properties of nc-Si.

This investigation has resulted in the development of a device level simulator which predicts quantum efficiency and voltage-current character for nc-Si/a-Si systems. These performance measures are calculated as functions of input photon energy. A number of different interactions were combined to completely characterize the device: optical scattering and absorption; creation of excitons and charge carriers; electrostatic fields; and drift-diffusion of charge carriers.

Objectives & Methods

- **Focus Goals**
  - Device response for nc-Si as function of nc size
  - Optimize short circuit current (J_sc) using nc size
- **Broader Impact**
  - Offer design guidance for nc-Si/a-Si composites
- **Nanocrystalline Silicon (nc-Si) Properties**
  - Band-gap 1.1 eV
  - Stable under light illumination
  - High carrier mobility
  - Amorphous Silicon (a-Si) Properties
  - Band-gap 1.7 eV
  - Degradation under light illumination
  - Low doping efficiency
  - Low carrier mobility
- **Device Simulator:** COMSOL Multiphysics
- **nc-Si quantum dots embedded in a-Si intrinsic region**
- **Volume fraction fixed at 50%**

References/Acknowledgements

Arun Madan, MRS Systems, Golden, CO – for providing resources on silicon quantum dots.


COMSOL Multiphysics version 3.5a (3.5.0.03) of 12-03-2008. COMSOL; Stockholm, Sweden.


SCAPS version 2.8.06 (“SCAPS2806”) of 2-26-2010. The University of Gent (“Belgium”). Department ELIS. Marc Burgelman, Koen Decock, Johan Verschraegen, Stefaan Degrave, Alex Namegara.