Analytical Approach to 3D Device Modeling of Nanoarchitectures for Solar Energy Conversion

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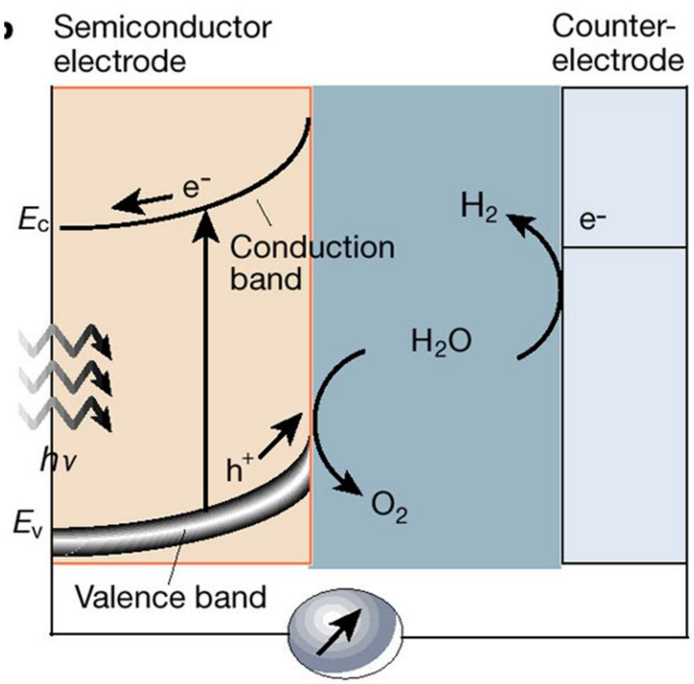
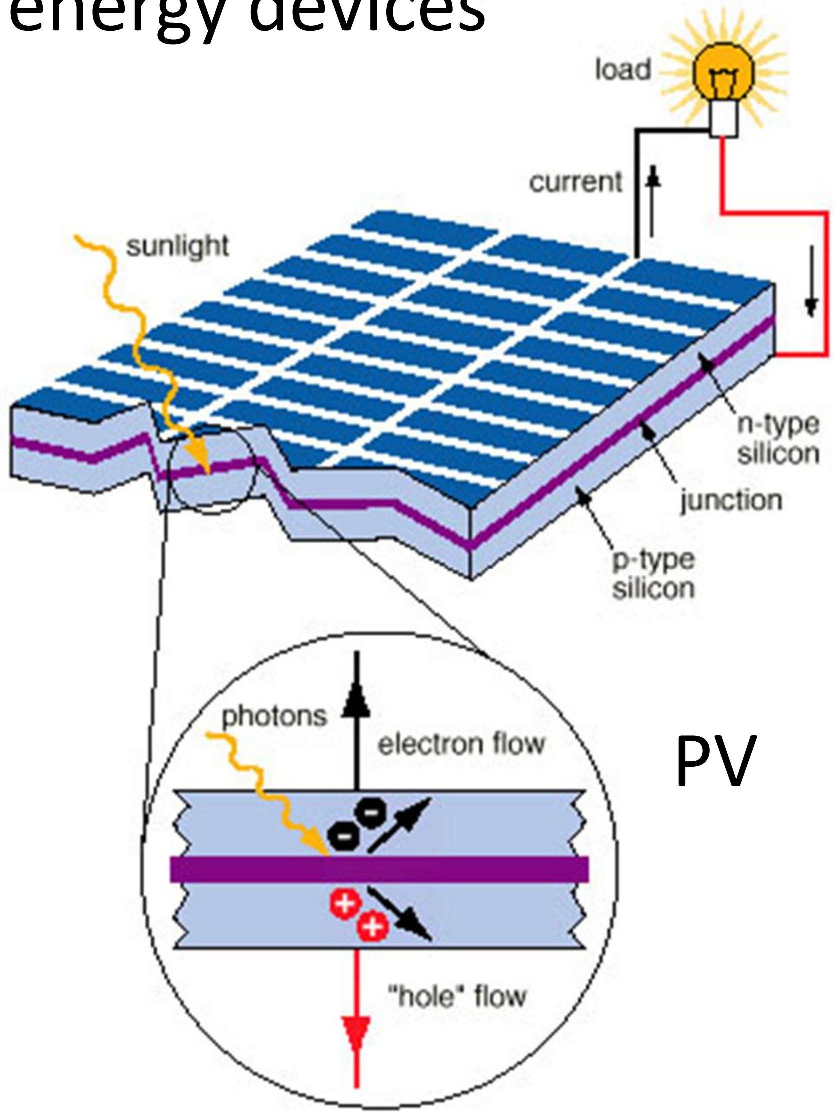
Renewable energy devices

PEC



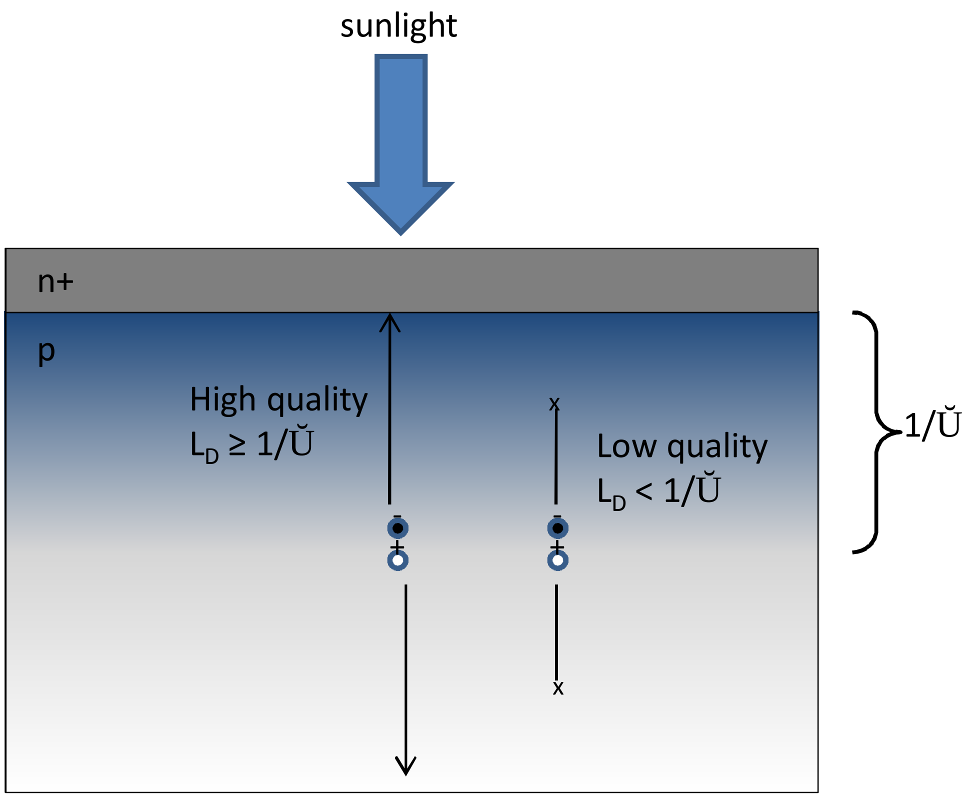
M. Grätzel, *Nature,* 414, 338 (2001).



PV

http://solar-module-panels.com/pv/solar-electricit/solar-cells/

Carrier collection in planar devices



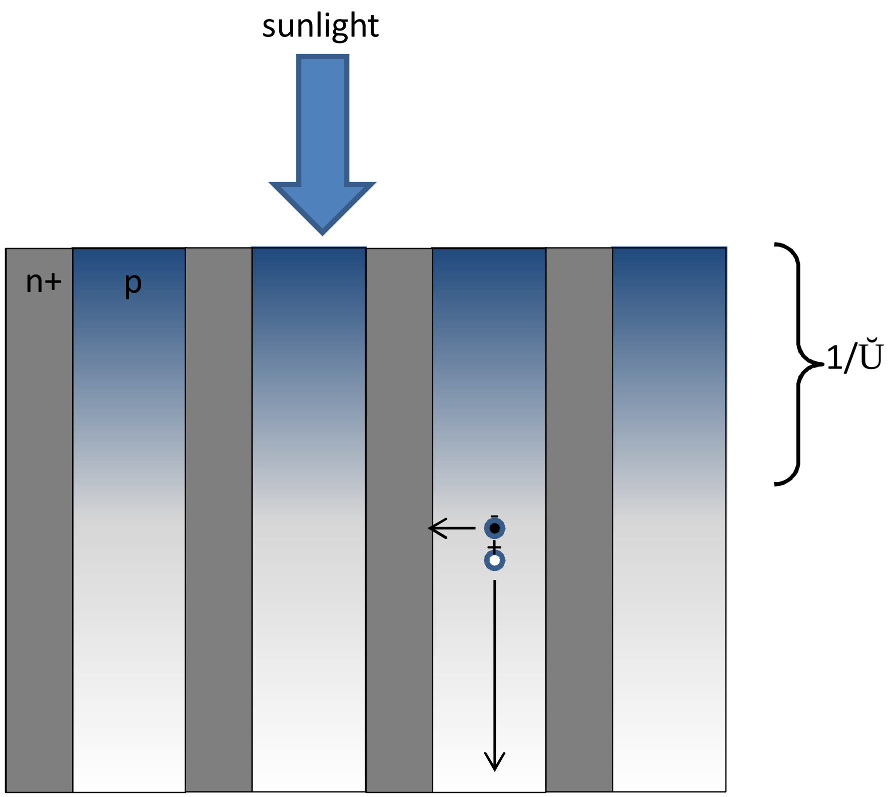
Diffusion length of minority carriers needs to be longer than the absorption depth for efficient carrier collection.

Problem: High quality materials are expensive. As for cheaper low quality materials, L_D is nanoscale.

Solution: Consider vertical nanojunctions to decouple absorption from collection.

Relevant to PEC as well.

Carrier collection in vertical junctions

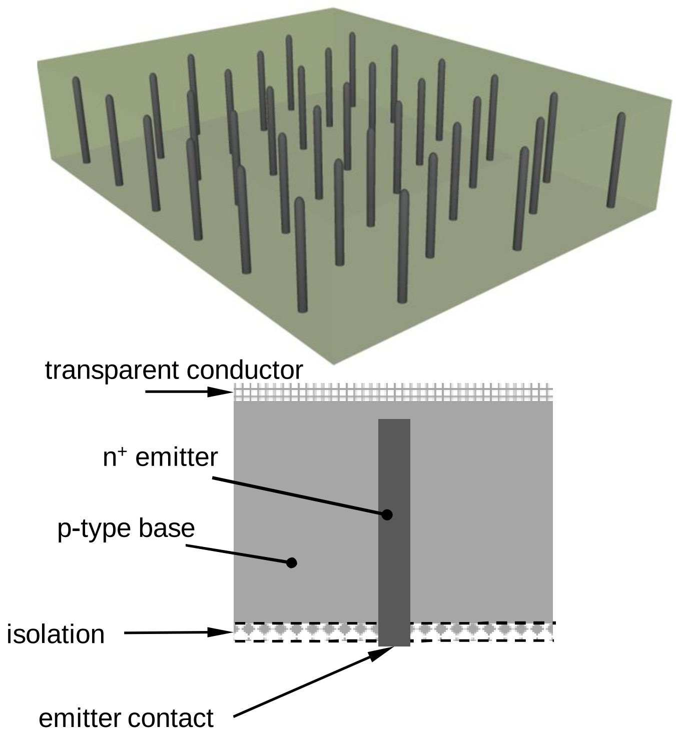


- Diffusion length of minority carriers no longer needs to be greater than the absorption depth for efficient carrier collection.
- Low-quality materials can be made more efficient.
- Since L_D is nanoscale, junction spacing should be nanoscale.
- To maximize benefit, we need to consider 3-D interdigitated nanojunctions.

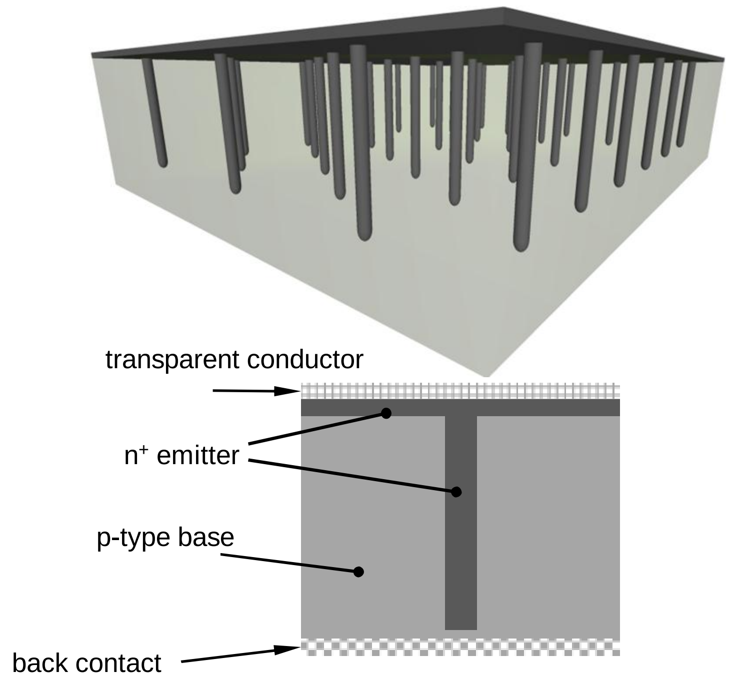
New 3D interdigitated designs reported

Note that electronic communication between junctions

1. Point-contact nanojunctions



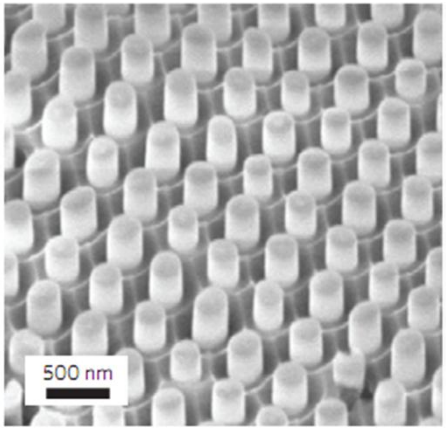
2. Extended nanojunctions

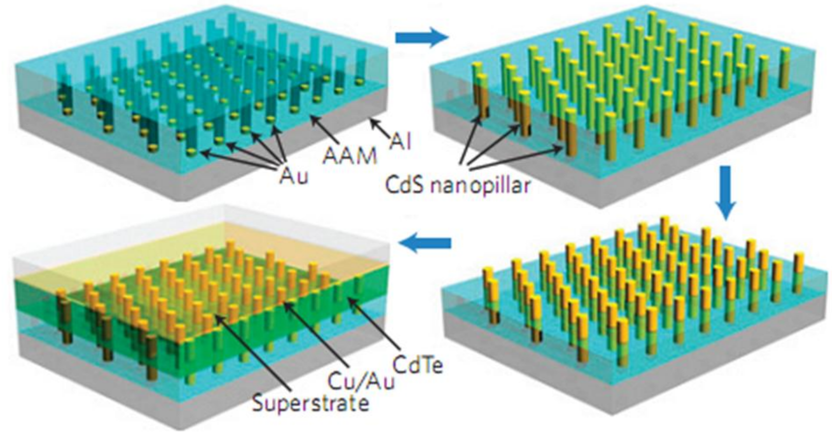


A. Wangperawong, S.F. Bent, *Appl. Phys. Lett.* **98**, 233106 (2011).

Experimental interdigated devices

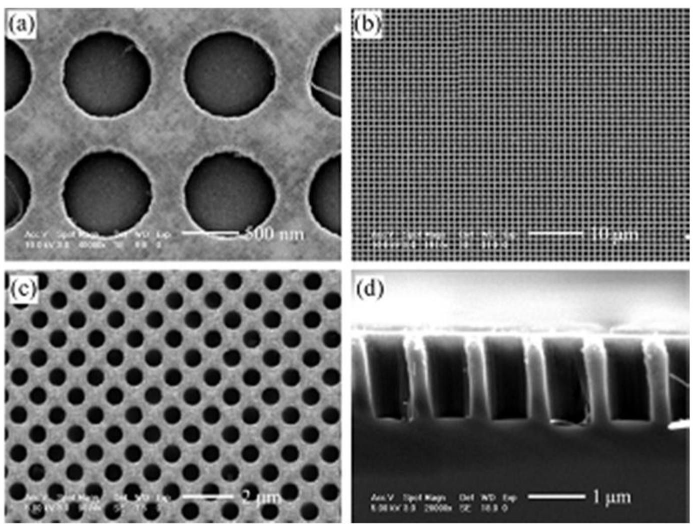
1. Point-contact nanojunctions

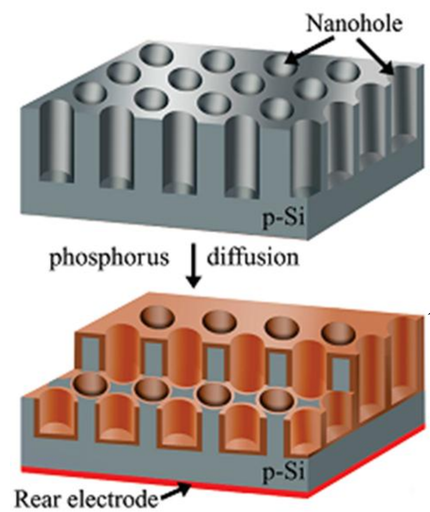




Fan, *et al.*, *Nature Mater.* 8, 648 (2009).

2. Extended nanojunctions



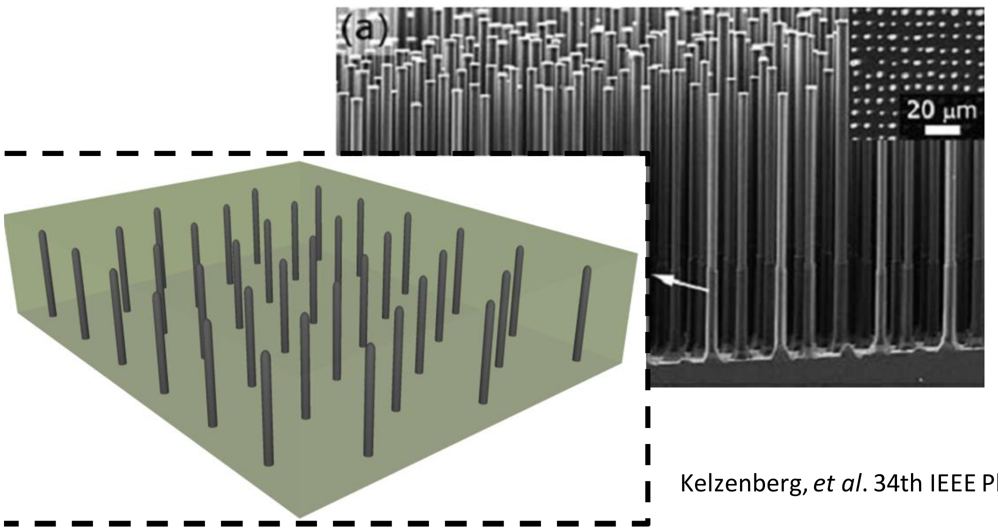


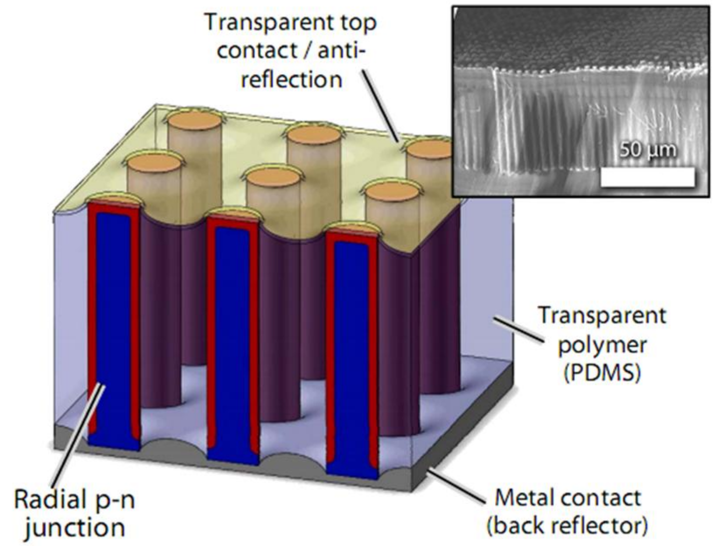
In place of n^+, electrolyte can be there for PEC

Peng, *et al.*, *J. Am. Chem. Soc.*, 132 (20), 6872 (2010).

Modeling beyond isolated nanojunctions

4. Isolated radial nanojunctions





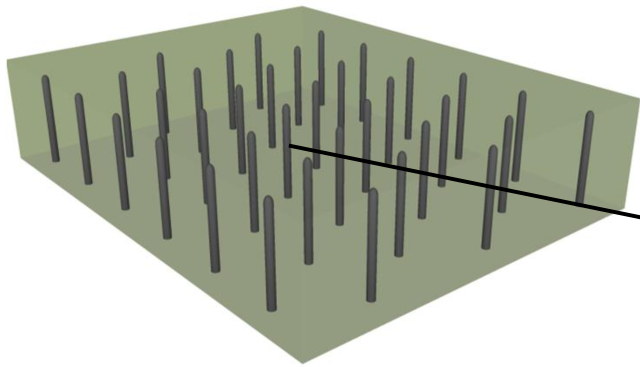
Kelzenberg, *et al*. 34th IEEE Photovoltaic Specialists Conference. IEEE , New York, pp. 391 (2010).

Limited 3D modeling work reported thus far

- Only on isolated radial junctions, i.e. nanowires.
  - Interdigitated design ≠ isolated radial junctions.
- Should consider 3D carrier collection – computationally expensive if numerical
- Is nano better than planar? Which nano is the best?
  - Depletion region lifetime greater than bulk lifetime + operate in full depletion
  - Not likely, not generally applicable

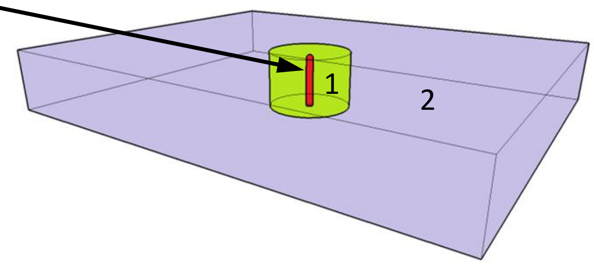
Modeling Approach

1. Point-contact nanojunctions

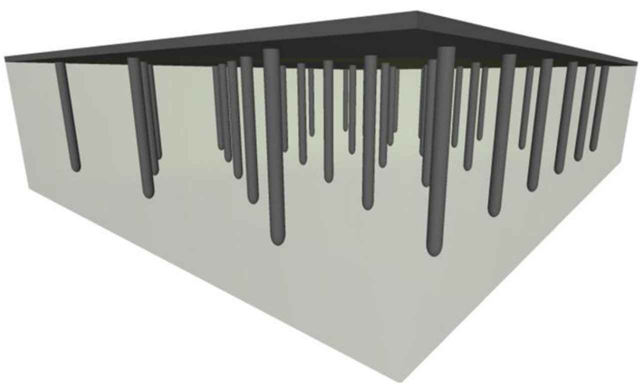


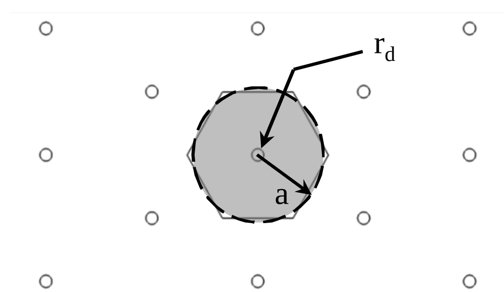
Analytical approach using effective medium approximation to solve diffusion-collection problem in 3-D:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \varphi_m}{\partial r}\right)+\frac{\partial^2 \varphi_m}{\partial z^2}-\frac{1}{L_m^{\ 2}}\varphi_m=0 \qquad m=1,2$$



2. Extended nanojunctions



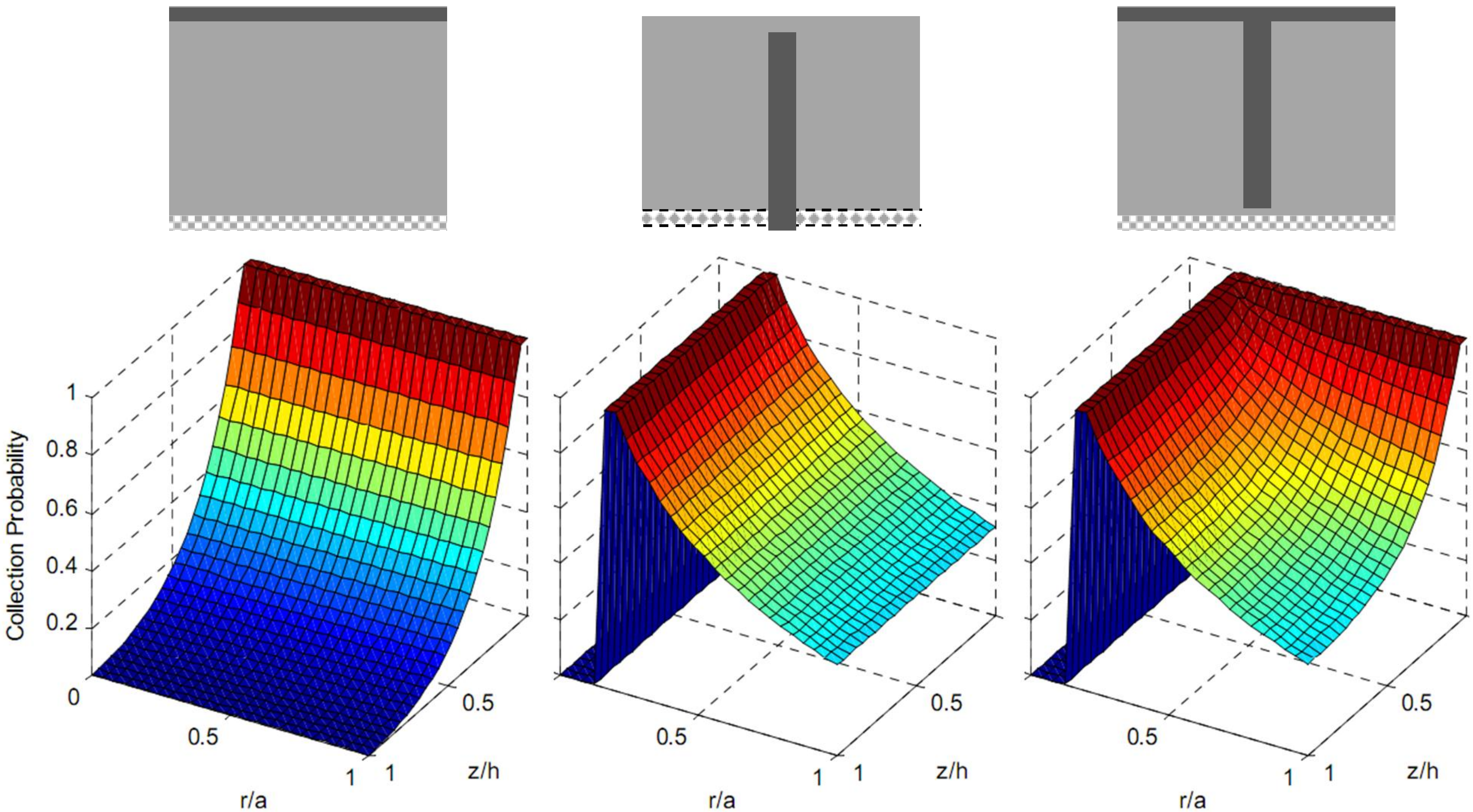


Boundary conditions due to continuity:

$$\varphi_1(r=a,z)=\varphi_2(r=a,z)$$

$$\left.\frac{\partial \varphi_1}{\partial r}\right|_{r=a}=\left.\frac{\partial \varphi_2}{\partial r}\right|_{r=a}$$

Collection Probability Distributions



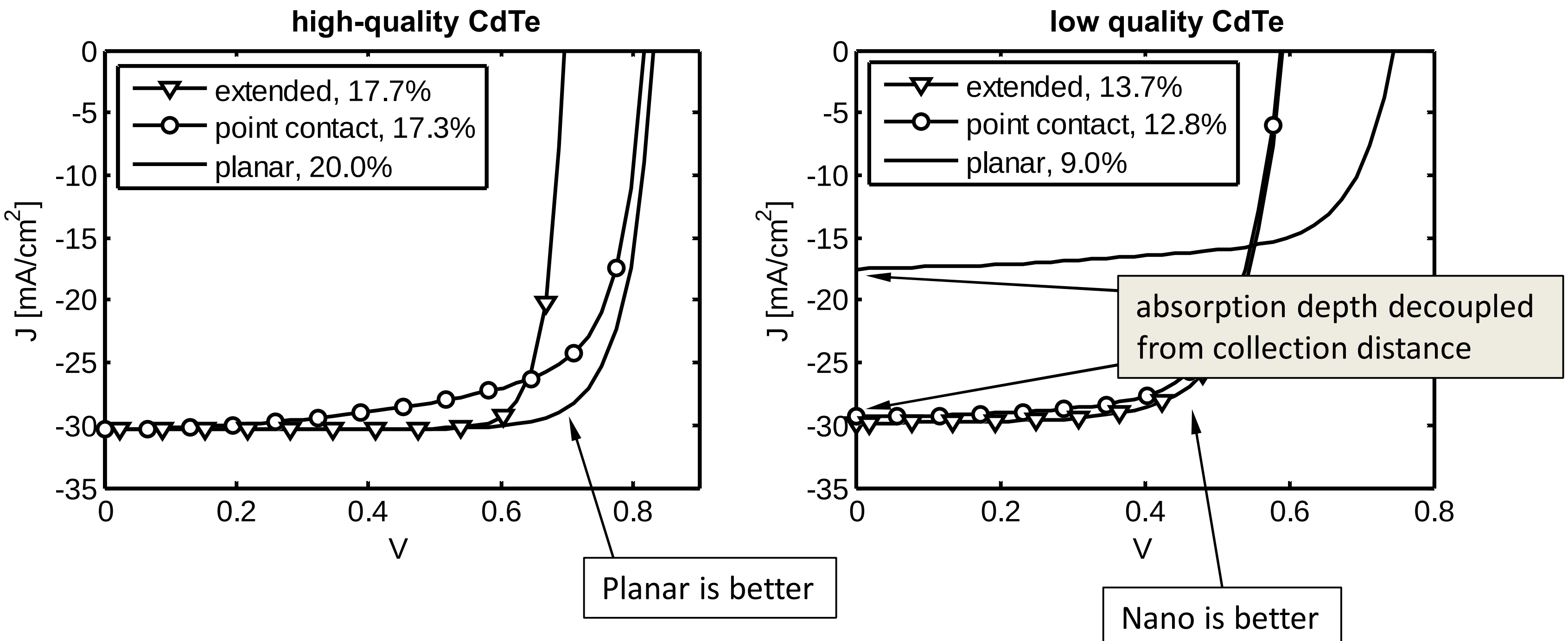
Application to PV

1. Calculate the depletion regions
2. Solve diffusion problem for carrier collection throughout device
3. Calculate the photocurrent
4. Relate carrier collection to minority carrier distribution throughout device
   - Calculate the ideal dark current
   - Calculate the depletion recombination current
5. Superimpose current contributions as a function of applied voltage to obtain overall I-V curves

CdTe/CdS devices, high vs. low

Property	High	Low	
Acceptor doping, N_a (cm^{-3})	$2x10^{14}$	$1x10^{17}$	higher doping
Electron mobility, μ_n (cm^2/Vs)	320	100	lower mobility
Electron lifetime, τ_n (ns)	1	$1x10^{-2}$	lower lifetime
Diffusion length, L_n (μm)	0.910	0.050	lower diffusion length

ÅZ. Fan, *et al.*, *Nature Mater.* 8, 648 (2009).
ÅR. Kapadia, *et al.*, *Appl. Phys. Lett.* 96, 103116 (2010).
ÅS. Adachi, Properties of Group-IV, III-V and II-VI Semiconductors, *Wiley*, West Sussex, England (2005).
ÅM. Gleockler, *et al.*, Numerical modeling of CIGS and CdTe solar cells: setting the baseline, *Proc. World Conf. Photov. Energy Conv.*, 3, 491 (2004).



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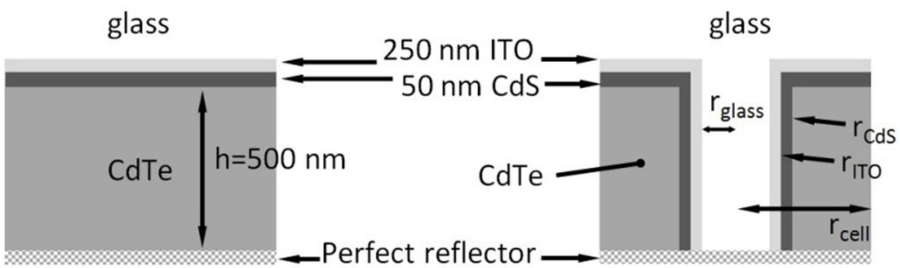
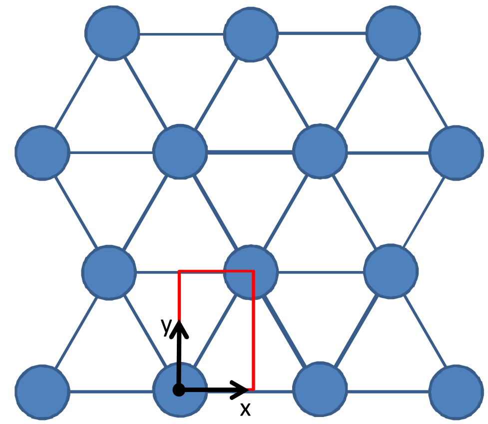
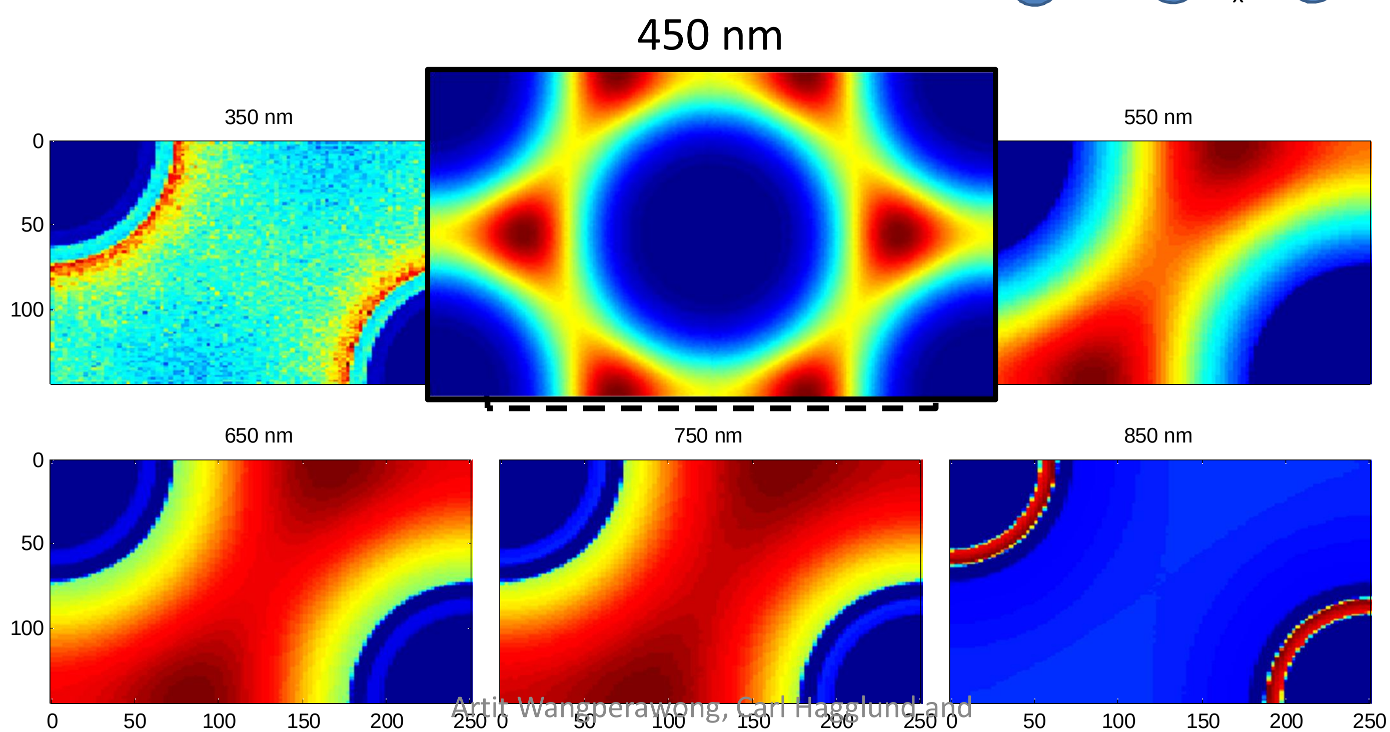
CdTe on Nanostructured SLG







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Conclusion

- We developed an analytical model for
  - diffusion in 3-D, interdigitated nanojunctions
  - both point-contact and extended architectures
  - any system involving diffusion, e.g. PEC, PV, etc.
- Nanojunctions can
  - decouple absorption depth from collection distance
  - improve performance of low quality PV absorbers, making use of inexpensive materials
- Modeling valuable for choosing the right nano-architecture
  - the efficiency of the extended nanojunction geometry is superior to other designs considered
  - point-contact nanojunction, isolated radial nanojunction, planar
- Various geometries and materials systems can be further explored
  - there could be an even better design out there

Acknowledgements

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