SAND2011-9014C

Record breaking solar cells: a materials perspective

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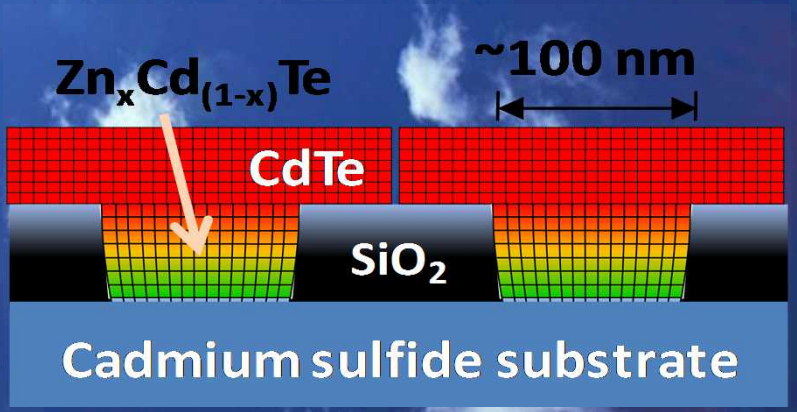
Xiaowang Zhou, Jose Chavez,
Brandon Aguirre, Jack Skinner,
Bruce Burckel, Carlos Sanchez,
and Gregory Nielson

4th Annual
Thin Film Solar Summit USA
December 2, 2011 - San Francisco, CA
4:00pm to 4:30pm



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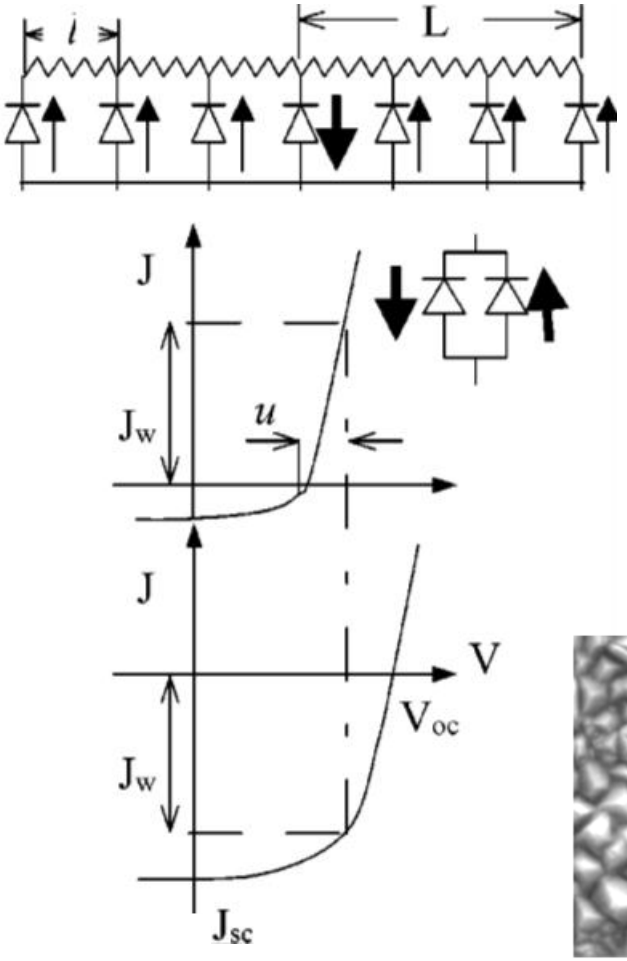
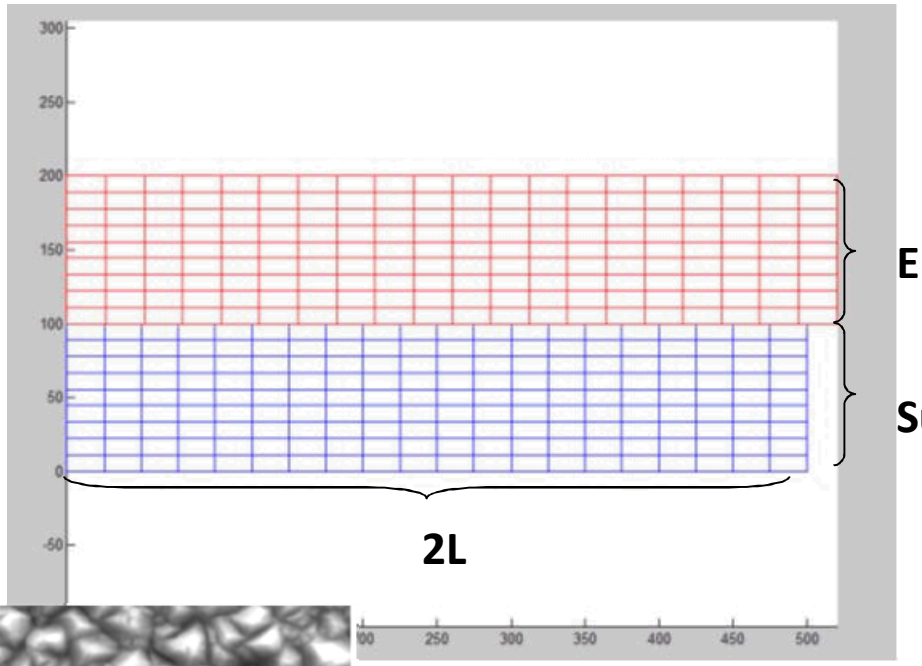
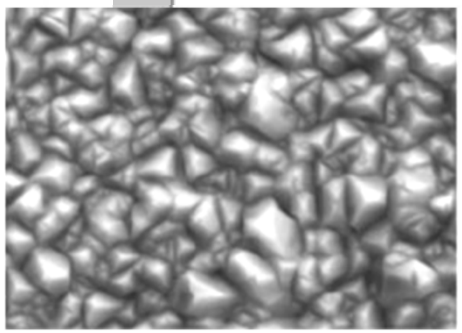
Non-uniformity and Lattice-mismatch lead to low efficiencies

*Non-uniformity → Loading losses



Lattice-Mismatch → Defects → Low V_{OC}

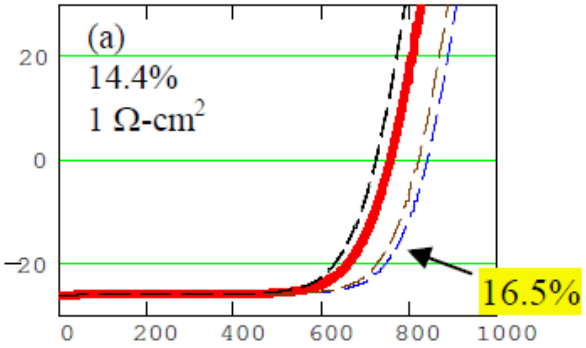




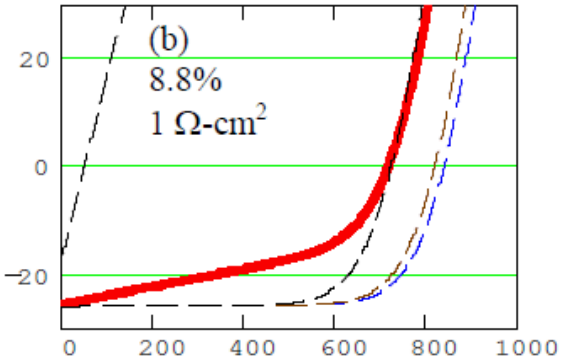
*V. G. Karpov, A. D. Compaan, and D. Shvydka, "Effects of nonuniformity in thin-film photovoltaics", Appl. Phys. Let. **80** (2002) 4256-4258.

Local inhomogeneity of the crystal grains is a dominant loss mechanism

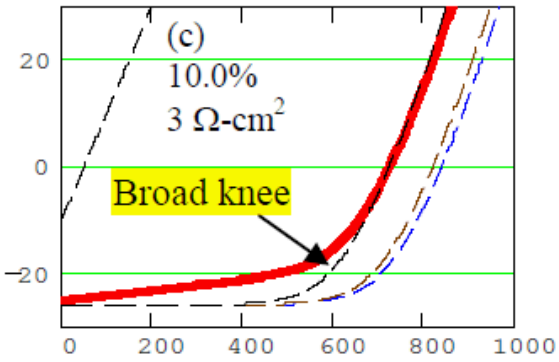
21-diode simulation



- Linearly vary I_s
- Low R_{series}



- 1 bad diode
- Low R_{series}



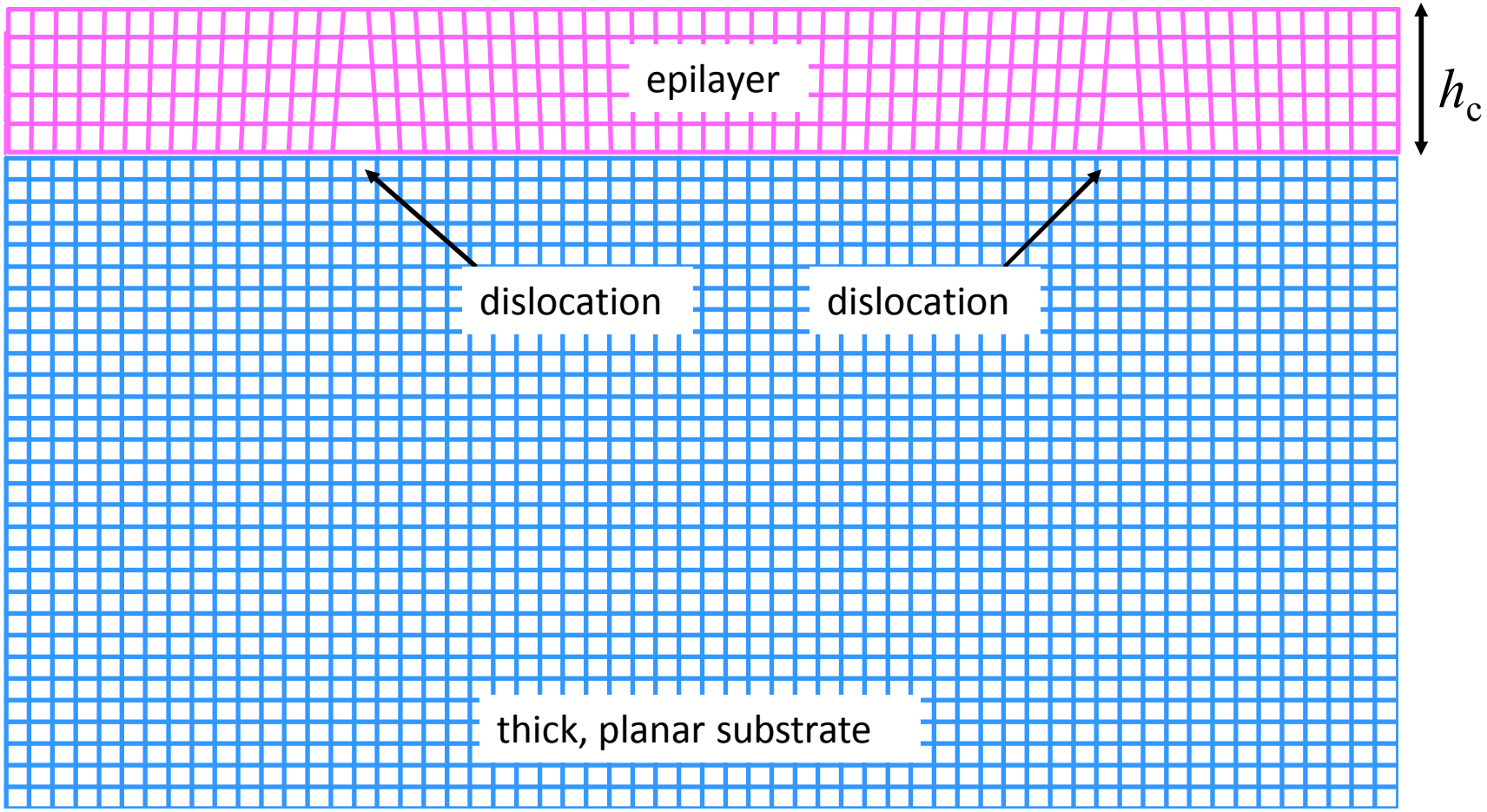
- 1 bad diode
- High R_{series}

Zubia, David; Romo, Luis; Cruz-Campa, Jose; Aguirre, Brandon; McClure, John; 34th IEEE Photovoltaic Specialists Conference , 2009 , pp: 001842 – 001845

Karpov, V.G., Compaan, A.D., and Shvydka, D. (2002). Effects of nonuniformity in thin-film photovoltaics. *Appl. Phys. Let.* 80, 4256-4258.

V. G. Karpov, A. D. Compaan, and D. Shvydka, "Effects of nonuniformity in thin-film photovoltaics", *Appl. Phys. Let*. **80** (2002) 4256-4258.

Strain energy due to lattice mismatch creates misfit dislocations

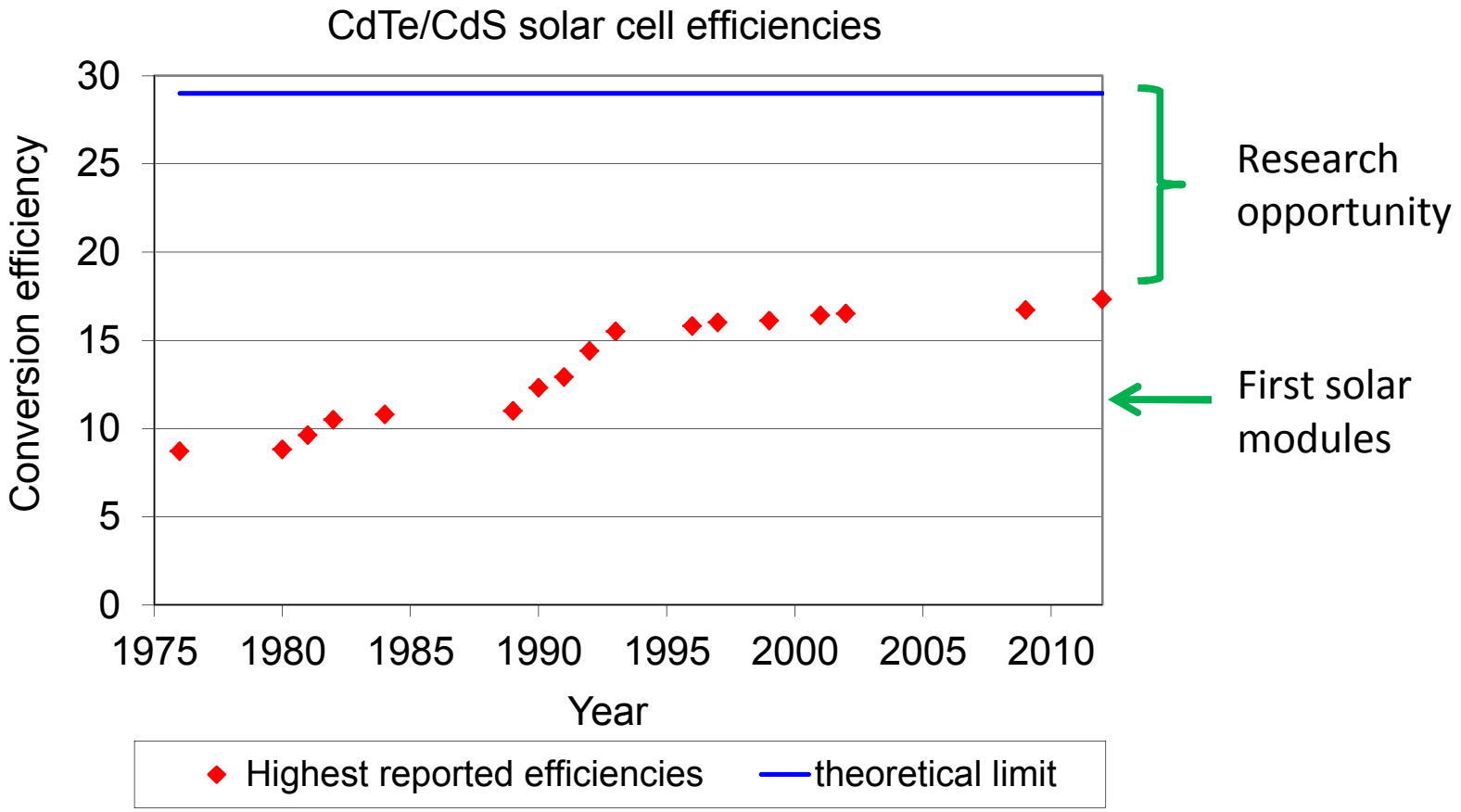


Misfit dislocations and grain boundaries reduce Voc

$$V_{OC} = \frac{E_g}{q} - \frac{kT}{q} ln(q^2 N_v p \frac{v_r^2}{J_L^2})$$

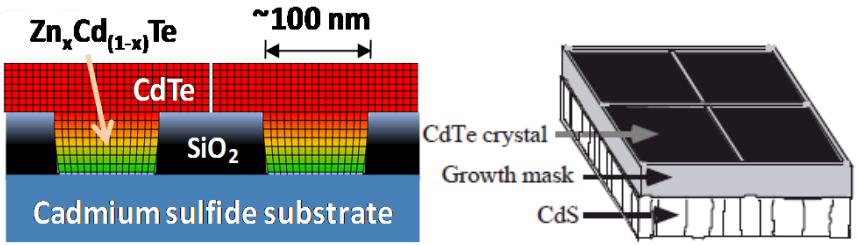
- *Defects increase the recombination velocity, v_r*
- *v_r reduces V_{oc}*

CdTe cell efficiencies have increased little over 18 years

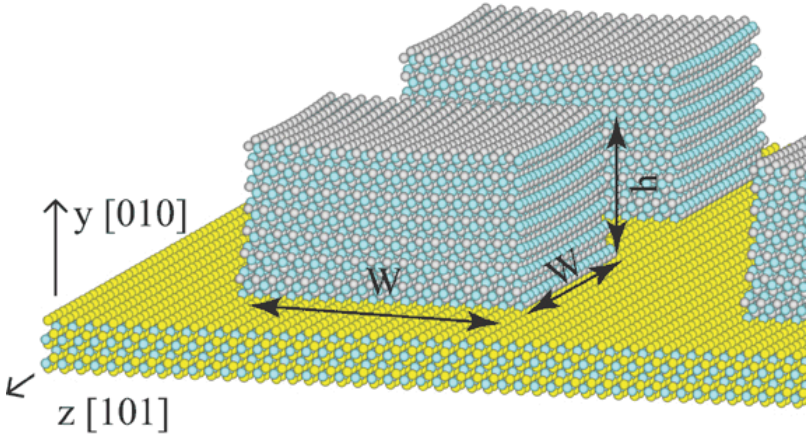


Outline

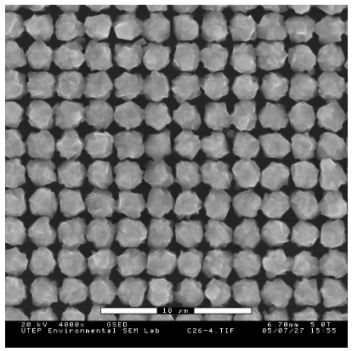
1. Proposed concept



2. Simulations

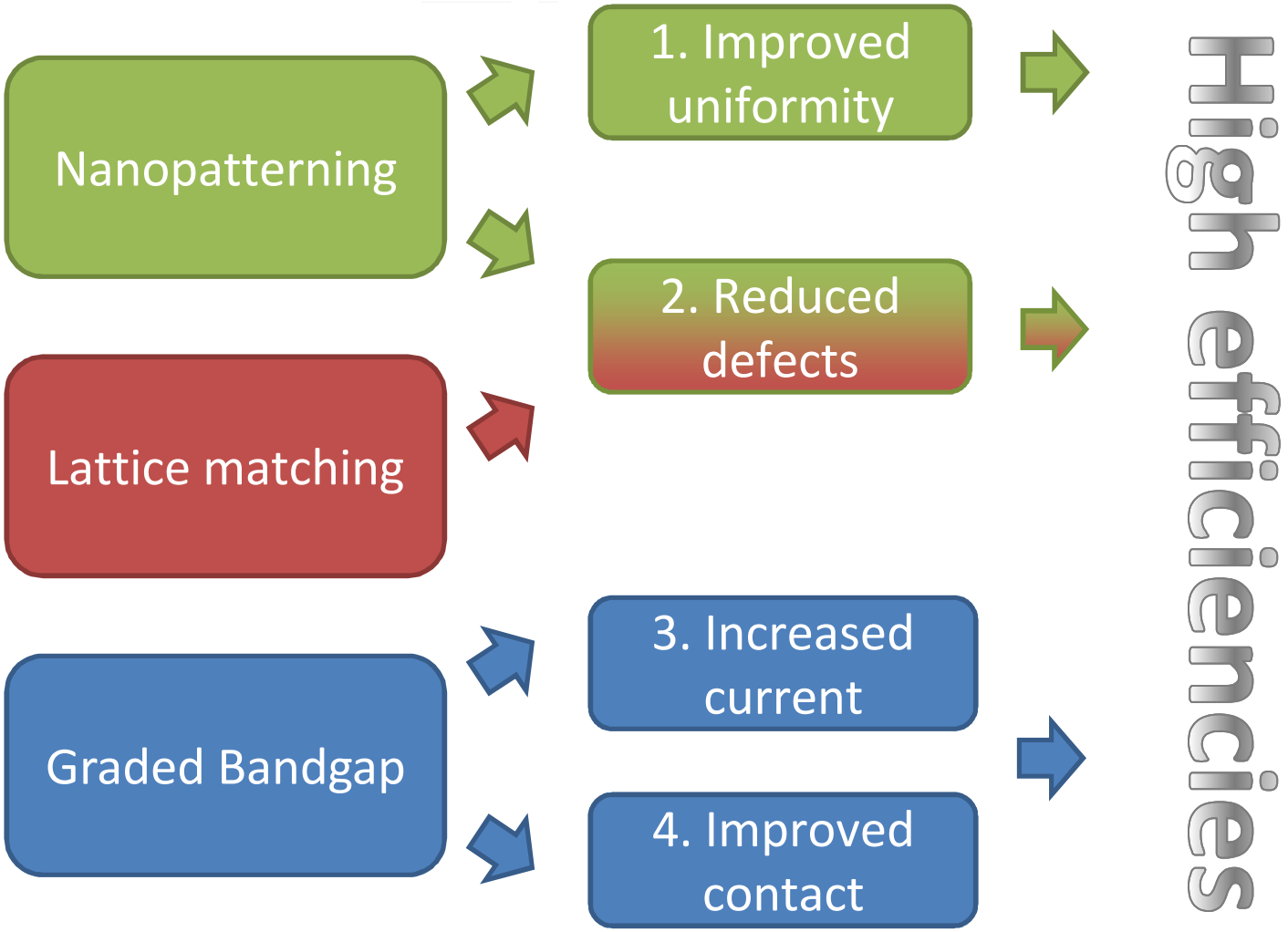


3. Initial Results



1. Proposed concept

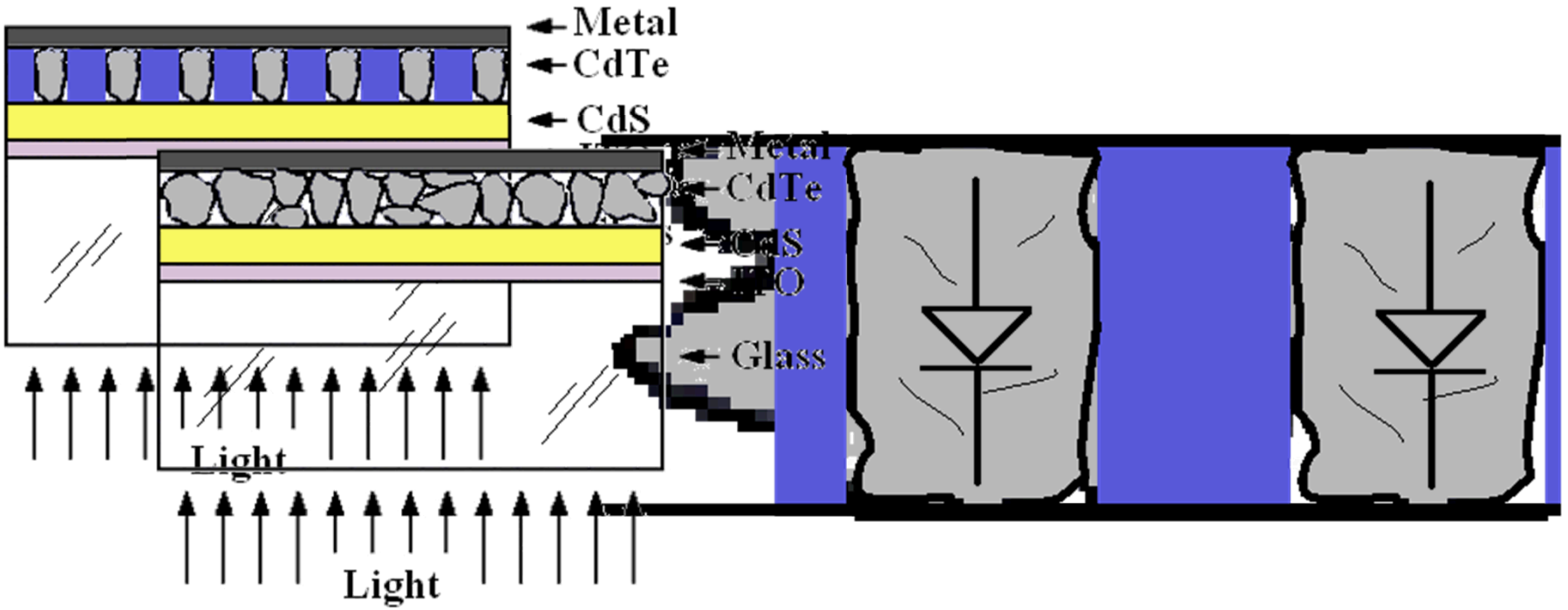
We propose nanopatterning and lattice matching to enhance cell performance



A patterned substrate can enhance uniformity

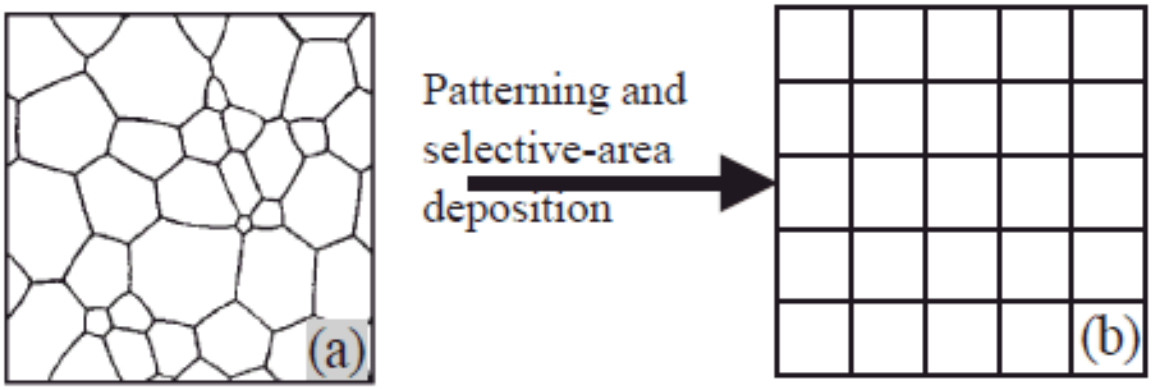
☒ Non-uniform growth on polycrystalline CdTe → efficiency losses.

☑ Improve uniformity by isolating grains.



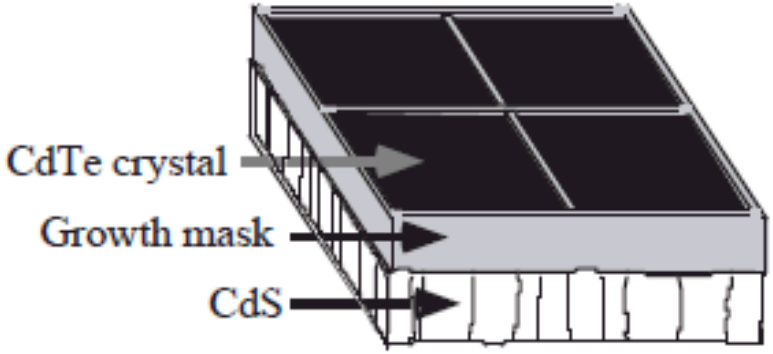
V. G. Karpov, A. D. Compaan, and D. Shvydka, "Effects of nonuniformity in thin-film photovoltaics", Appl. Phys. Let. **80** (2002) 4256-4258.

Nanopatterning can improve uniformity



Non uniform

Uniform

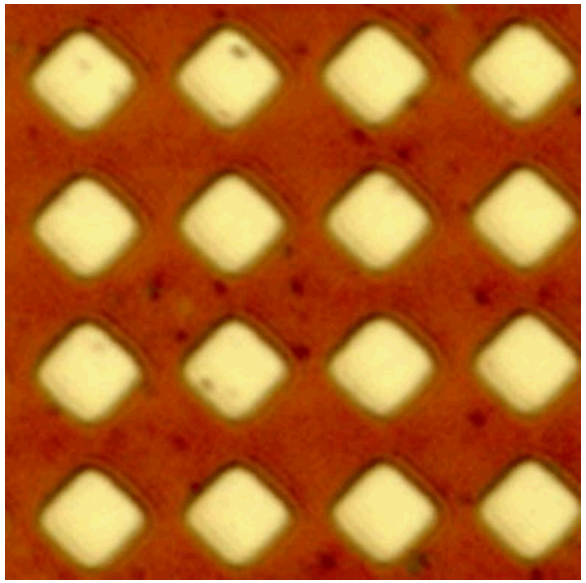


Controlled nucleation

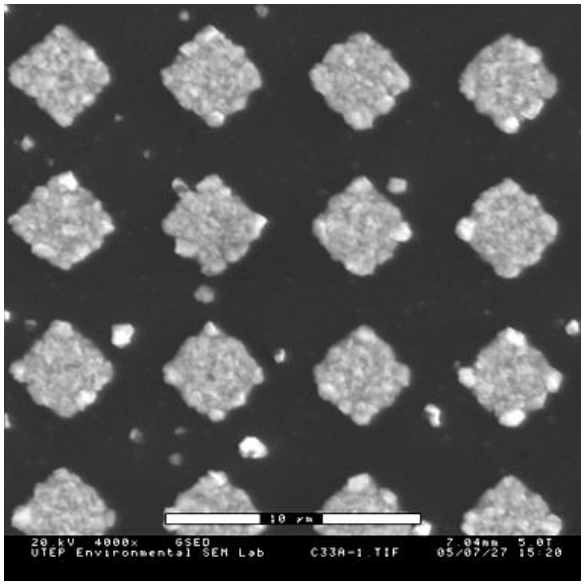
Javier Terrazas, Aaron Rodriguez, Cesar Lopez, Arev Escobedo, Franz J. Kuhlmann, John McClure, David Zubia, Ordered polycrystalline thin films for high performance CdTe/CdS solar cells, Thin Solid Films, Volume 490, Issue 2, IMRC 2004, 1 November 2005, Pages 146-153

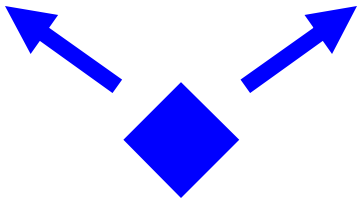
Growth mimics shape of pattern

- Patterned SiO_2



- Ordered CdTe

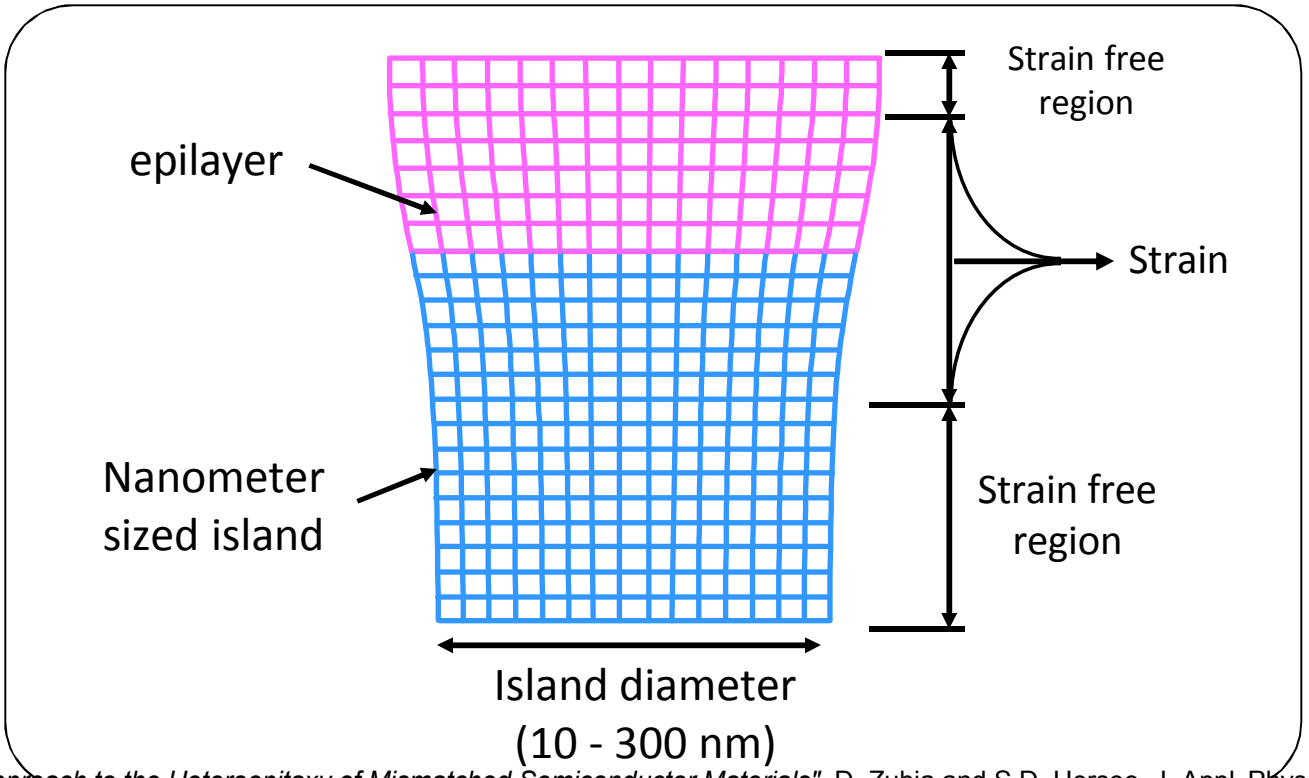




Diamond shape and size is mimicked

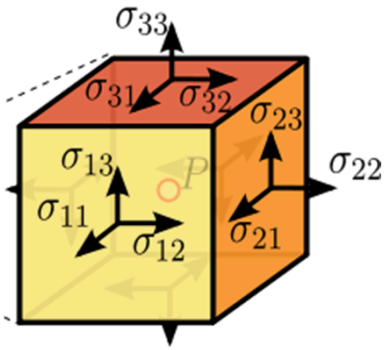
Nanopatterning reduces defects through nanoscale 3D strain relief

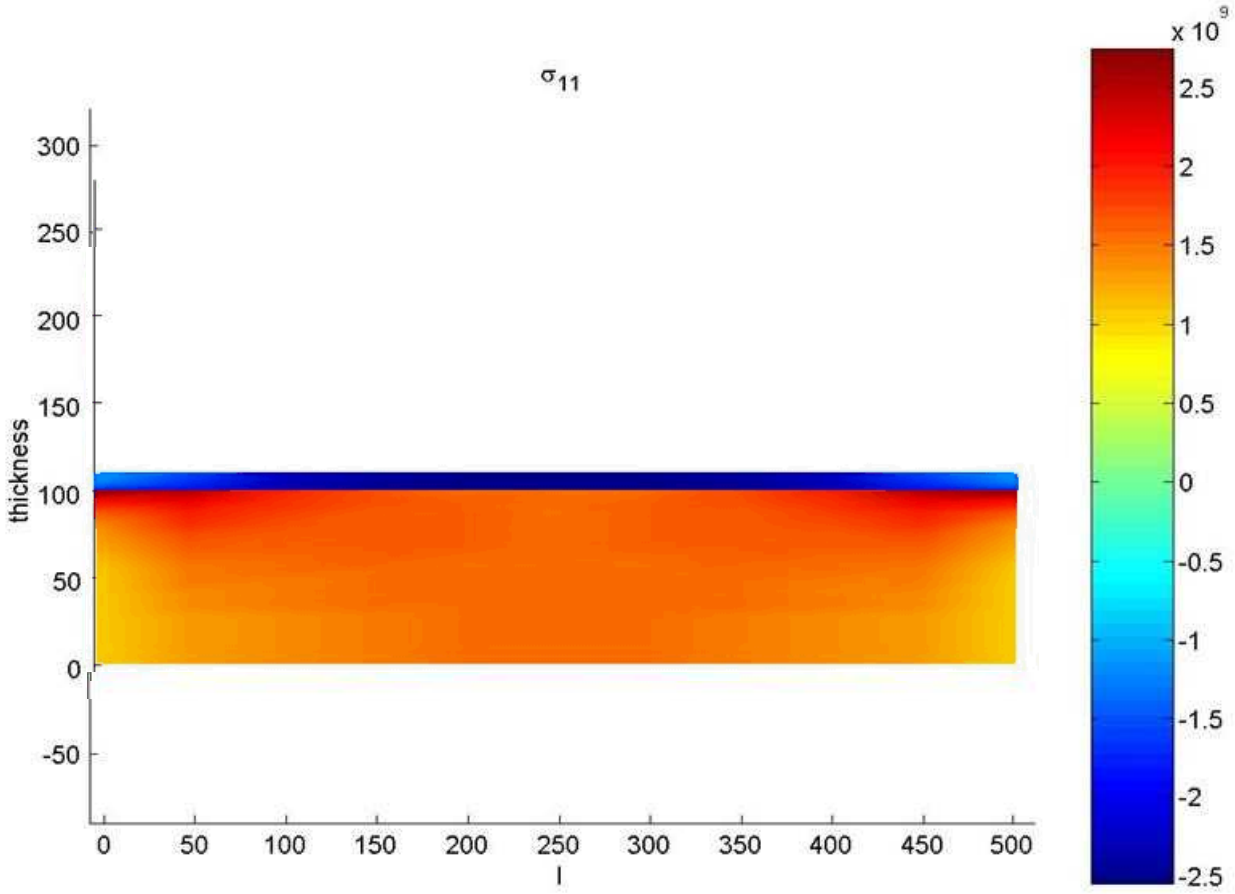
- Lattice mismatch is partly accommodated by substrate
- Strain decays exponentially away from the interface
- Epilayer is essentially strain-free beyond characteristic length of decay



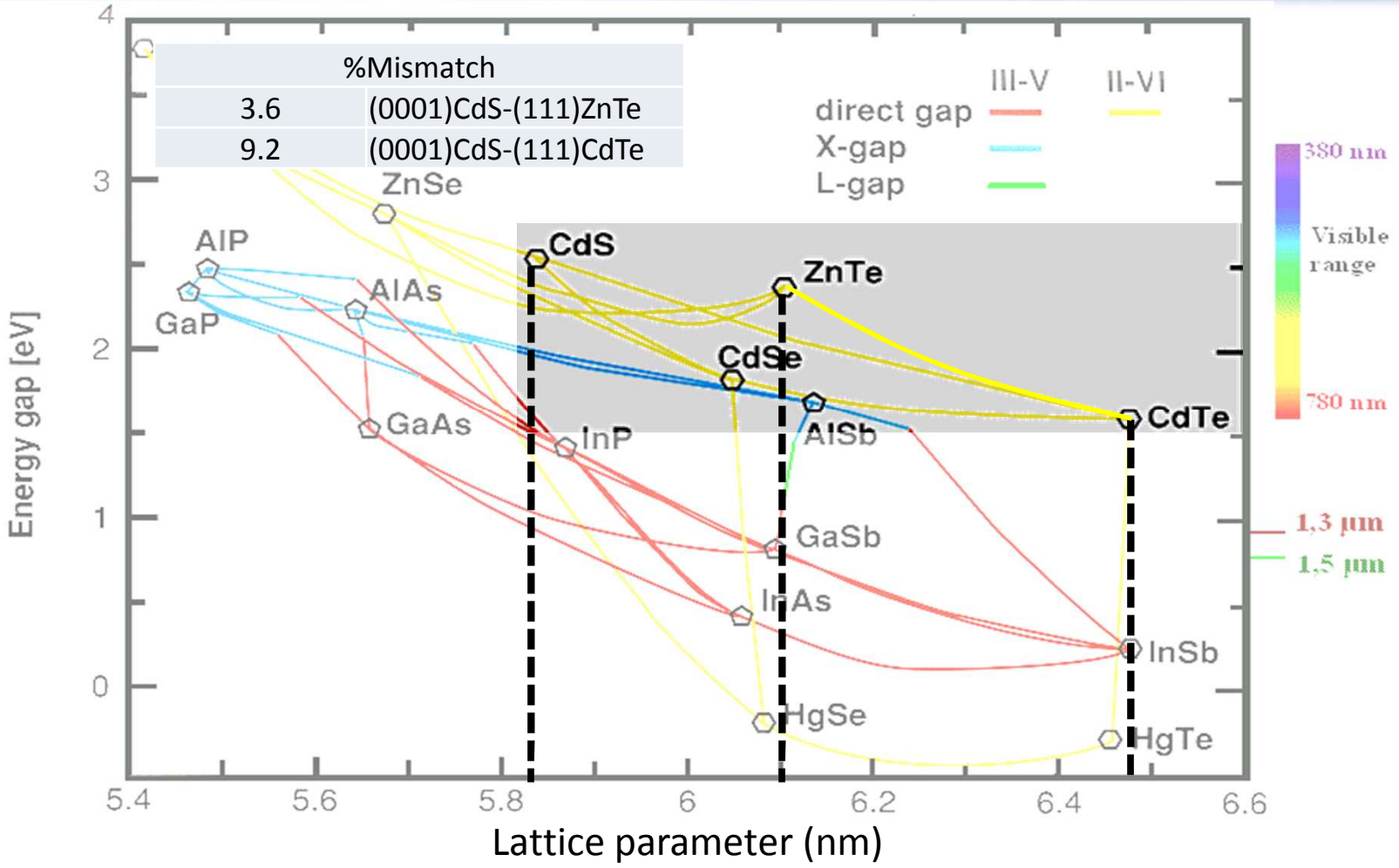
"Nanoheteroepitaxy: A New Approach to the Heteroepitaxy of Mismatched Semiconductor Materials", D. Zubia and S.D. Hersee, J. Appl. Phys., **85** (1999) 6492-6496

Finite element modeling shows strain partitioning

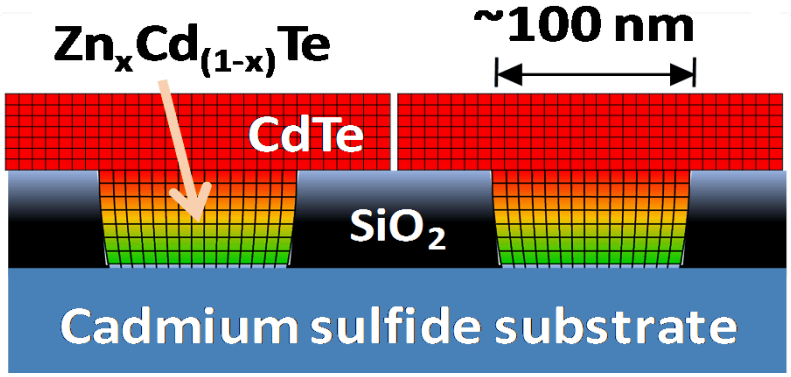




Lattice matching reduces defects even further



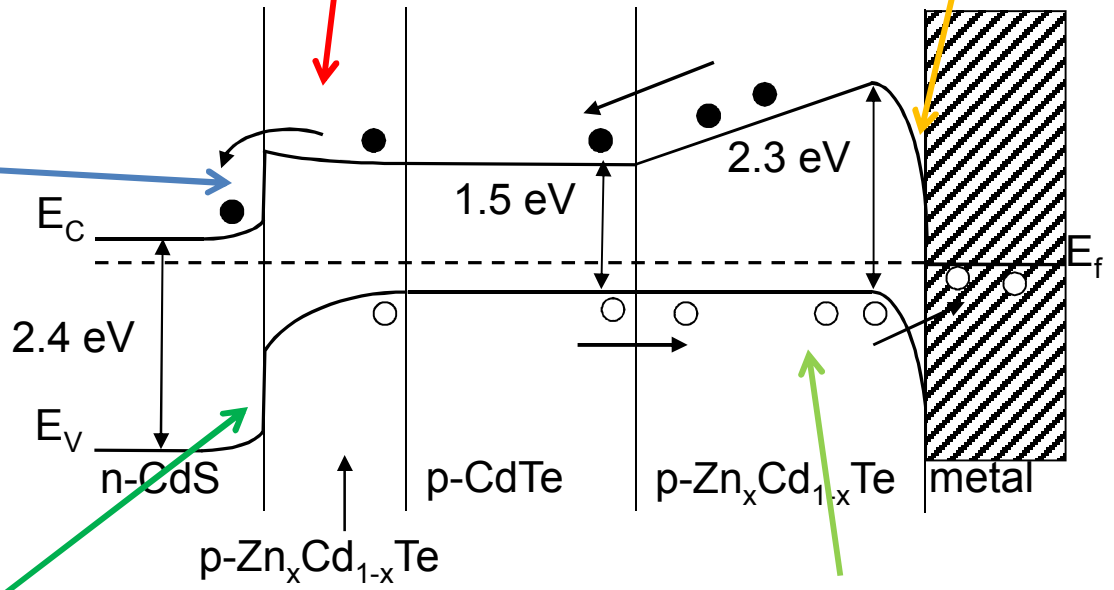
A graded bandgap can increase current and enhance contacts



Spatial variation of the band-gap can increase both J_{sc}

high level doping (10^{18} cm^{-3}) thus creating a tunneling junction with the metal electrode

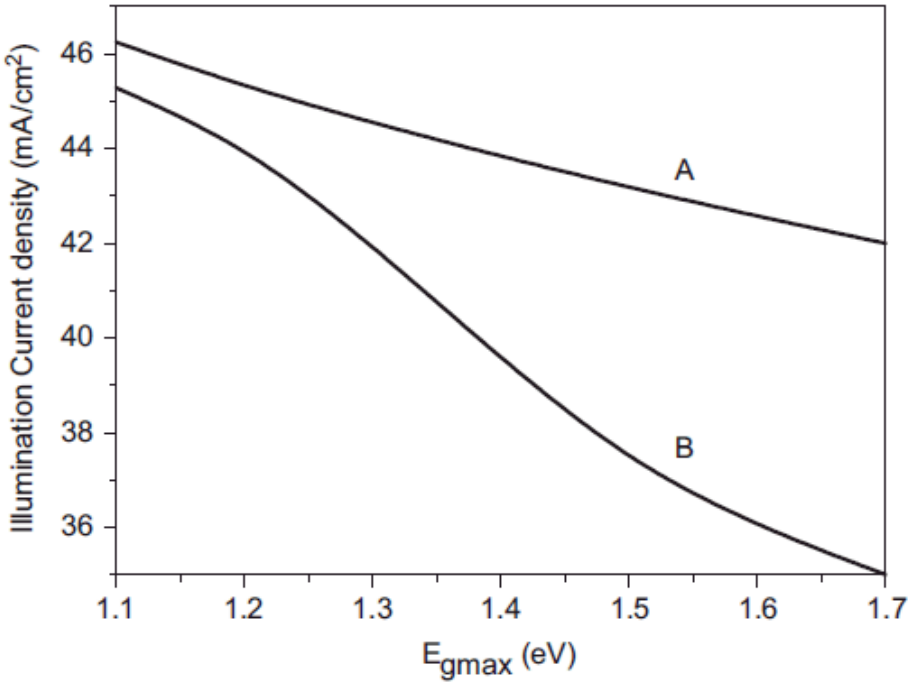
Reduced lattice mismatch



band offset enhances electron-hole charge separation

Graded bandgap creates a field along the structure

A graded bandgap can also increase current

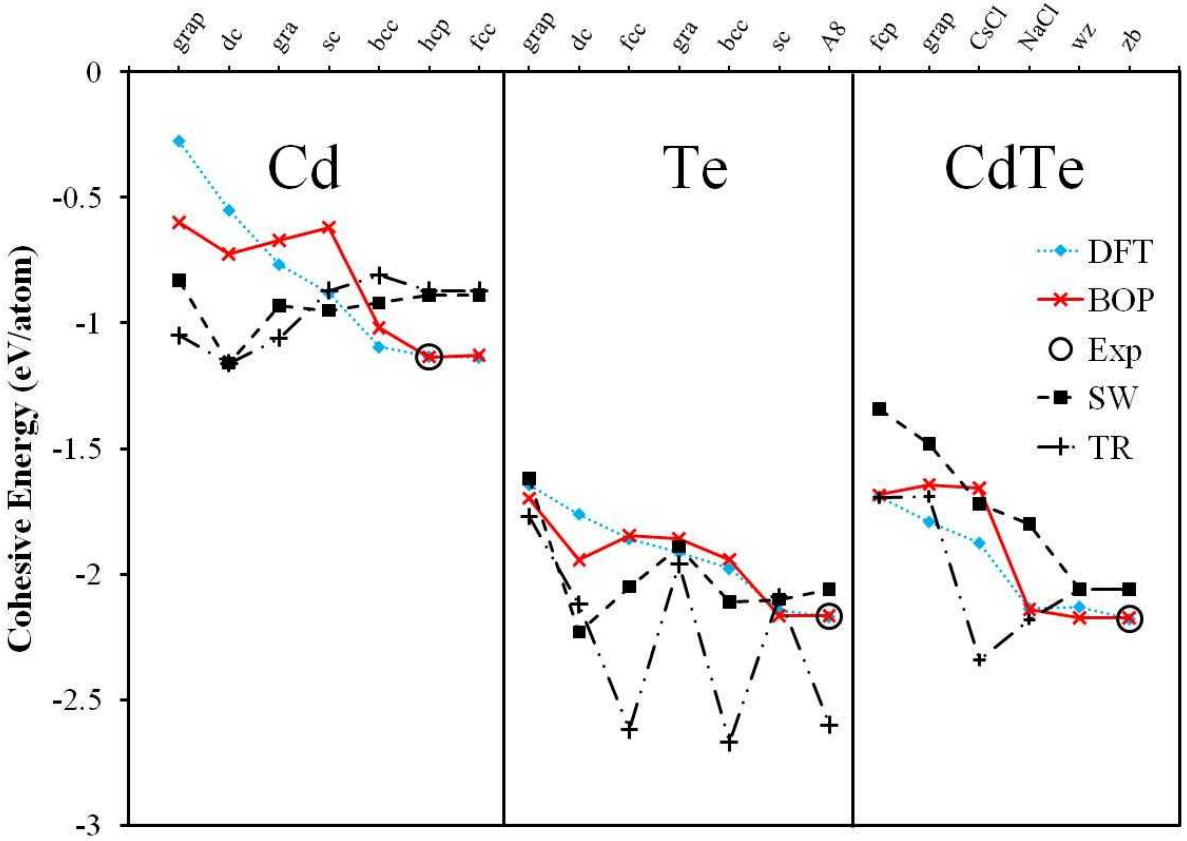


Illumination current density as a function of E_{gmax} with constant E_{gmin}=1eV and thickness d=3μm, for a cell that has an absorbing material with (A) linear band-gap variation, and (B) constant band-gap with the average E_g

Arturo Morales-Acevedo, Effective absorption coefficient for graded band-gap semiconductors and the expected photocurrent density in solar cells, Solar Energy Materials and Solar Cells, Volume 93, Issue 1, January 2009, Pages 41-44

2. Simulations

Our CdTe-BOP Captures Energy Trends of Many Cd, Te, and CdTe Phases

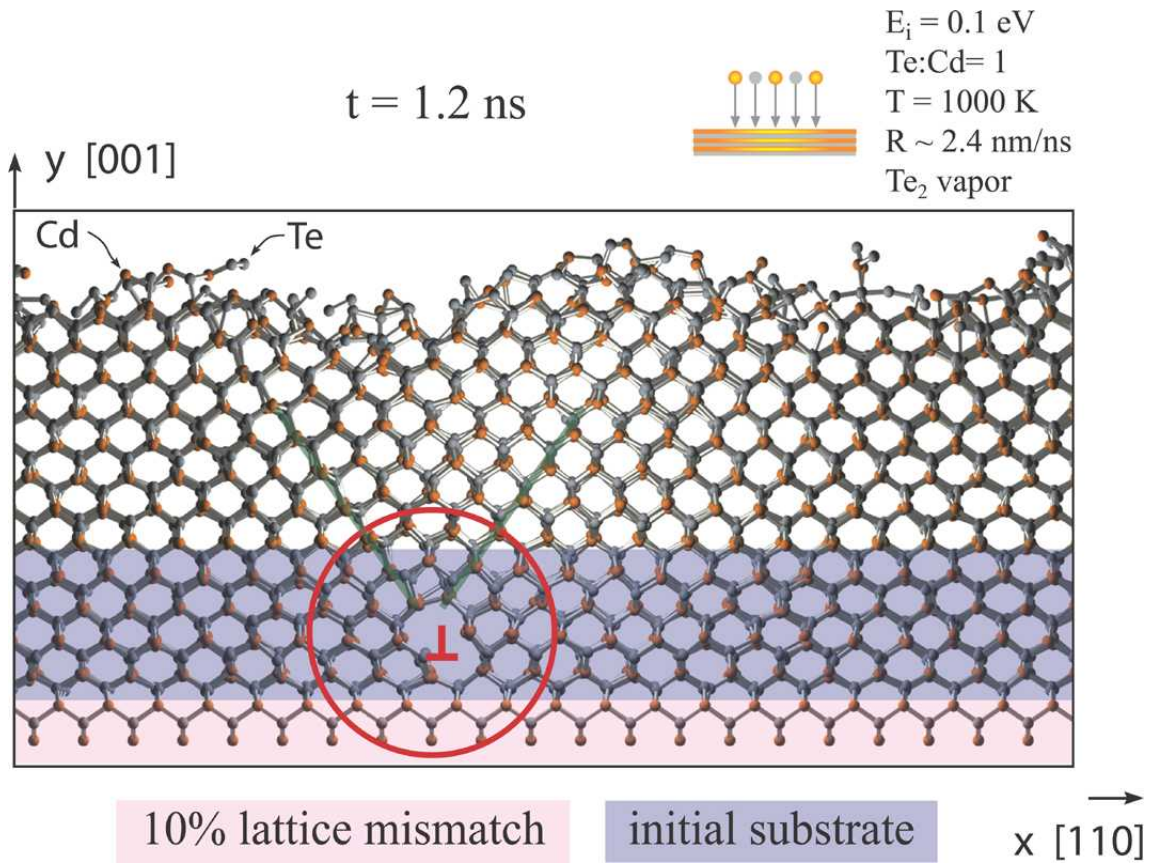


grap: graphene;
dc: diamond-cubic;
gra: graphite;
sc: simple-cubic;
bcc: body-centered cubic;
hcp: hexagonal-close-packed;
fcc: face-centered-cubic;
wz: wurtzite;
zb: zince-blende; etc.

DFT= Density Functional Theory
BOP= Bond order potential
Exp= Experimental
SW= Stillinger Weber
TR= Tersoff

1. D. G. Pettifor, M. W. Finnis, D. Nguyen-Manh, D. A. Murdick, X. W. Zhou, and H. N. G. Wadley, Mater. Sci. Eng. A, 365, 2 (2004).
2. D. G. Pettifor, and I. I. Oleinik, Phys. Rev. B, 59, 8487 (1999).
3. D. G. Pettifor, and I. I. Oleinik, Phys. Rev. Lett., 84, 4124 (2000).
4. D. G. Pettifor, and I. I. Oleinik, Phys. Rev. B, 65, 172103 (2002).
5. R. Drautz, D. A. Murdick, D. Nguyen-Manh, X. W. Zhou, H. N. G. Wadley, and D. G. Pettifor, Phys. Rev. B, 72, 144105 (2005).
6. D. A. Murdick, X. W. Zhou, H. N. G. Wadley, D. Nguyen-Manh, R. Drautz, and D. G. Pettifor, Phys. Rev. B, 73, 45206 (2006).

MD Simulations show the capability to simulate misfit dislocations

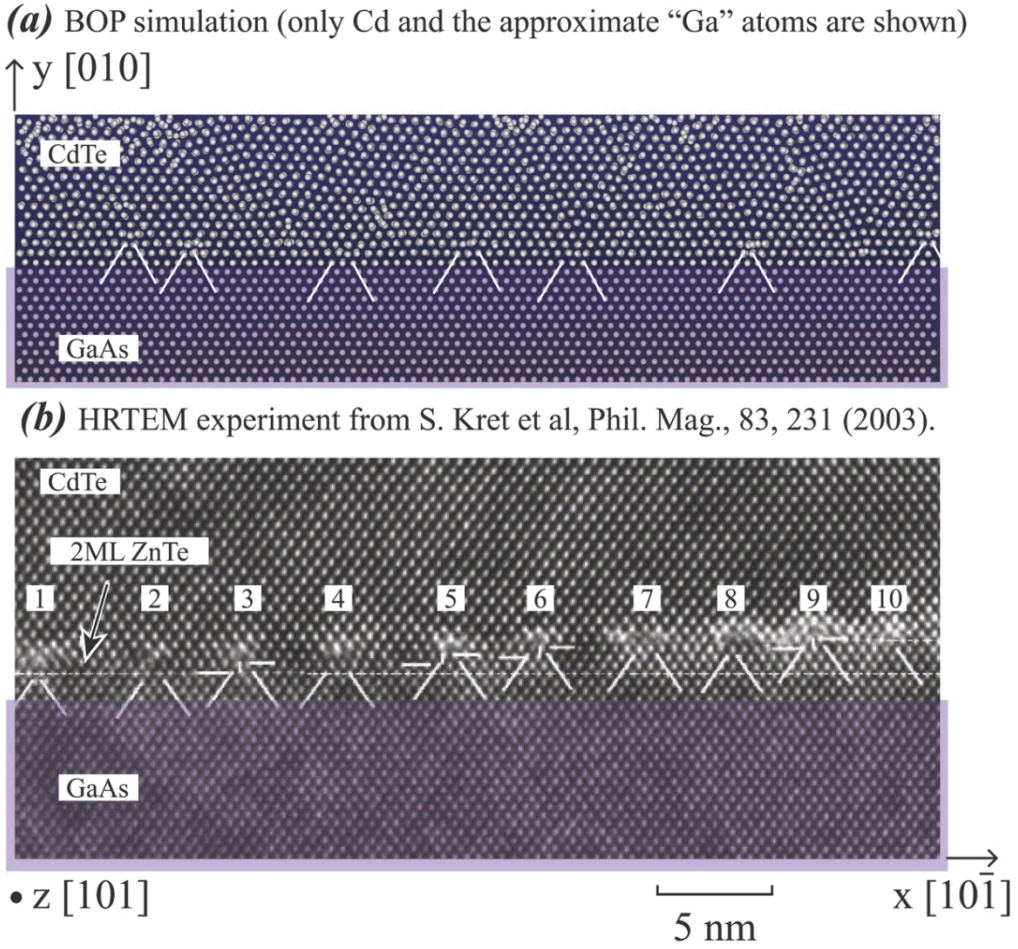


BOP-based MD

- Emerges to be a new, powerful method to study thin film growth
- Captures the crystalline growth of stoichiometric films (Cd/Te = 1) under non-stoichiometric, random vapor fluxes
- Reveals misfit dislocation formation

J. J. Chavez, D. K. Ward, B. M. Wong, F. P. Doty, J. L. Cruz-Campa, G. N. Nielson, V. P. Gupta, D. Zubia, J. McClure, and X. W. Zhou, Defect formation dynamics during CdTe overlayer growth, Unpublished

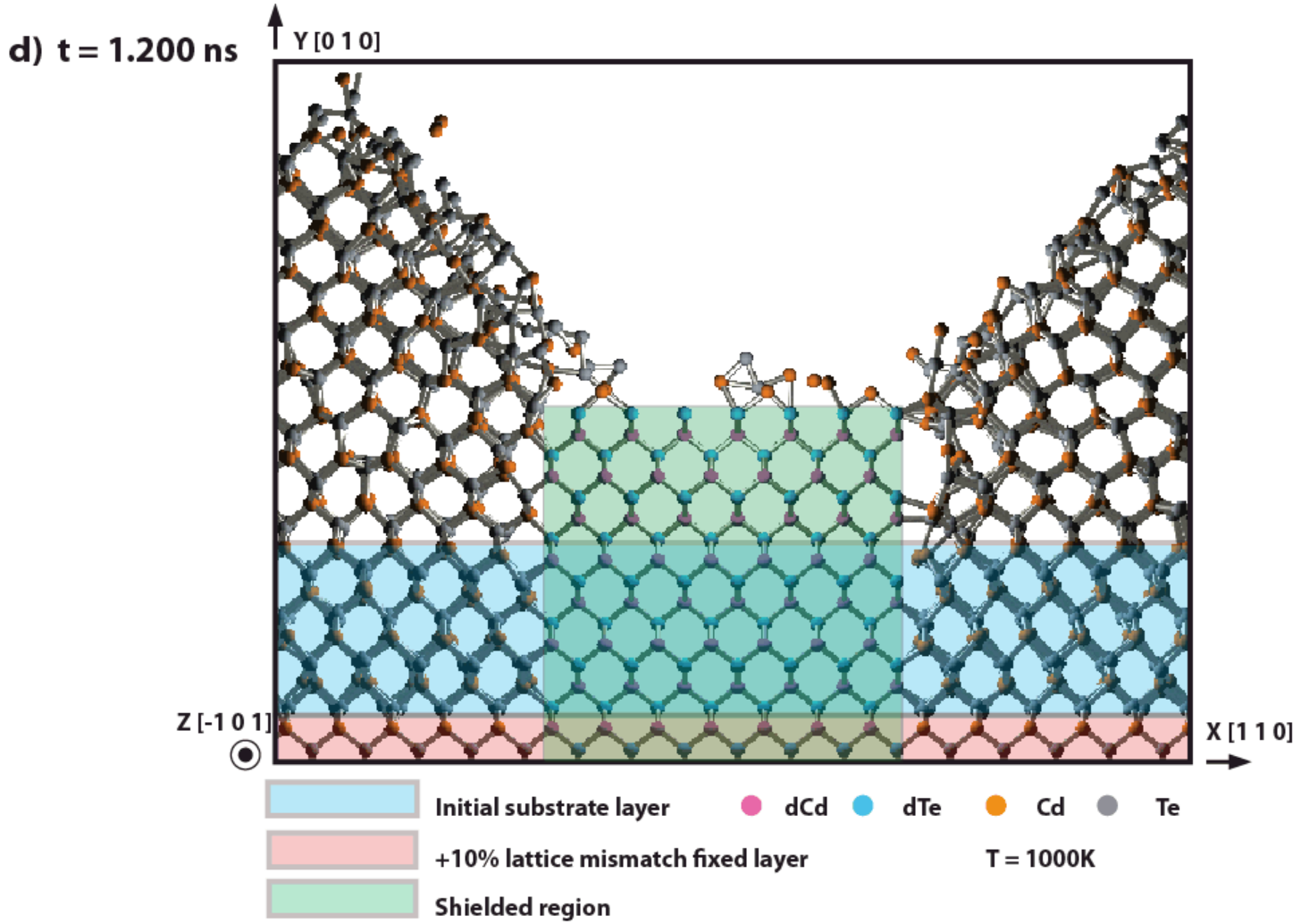
BOP of misfit dislocations in CdTe/GaAs Films are validated with experimental data



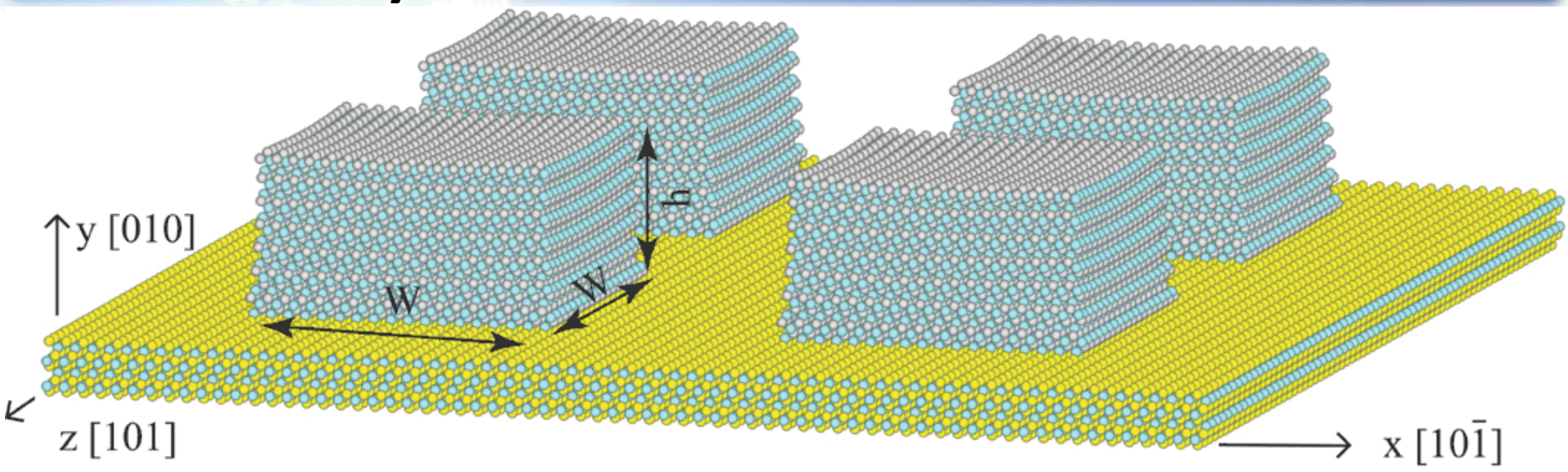
- BOP allows system energy as a function of dislocation spacing to be derived
- Minimization of system energy with respect to dislocation spacing leads to an equilibrium spacing around 3.8 nm, matching remarkably well with experiments

J. J. Chavez, D. K. Ward, B. M. Wong, F. P. Doty, J. L. Cruz-Campa, G. N. Nielson, V. P. Gupta, D. Zubia, J. McClure, and X. W. Zhou, Defect formation dynamics during CdTe overlayer growth, Unpublished

BOP has predicted selective growth of material in patterned substrates

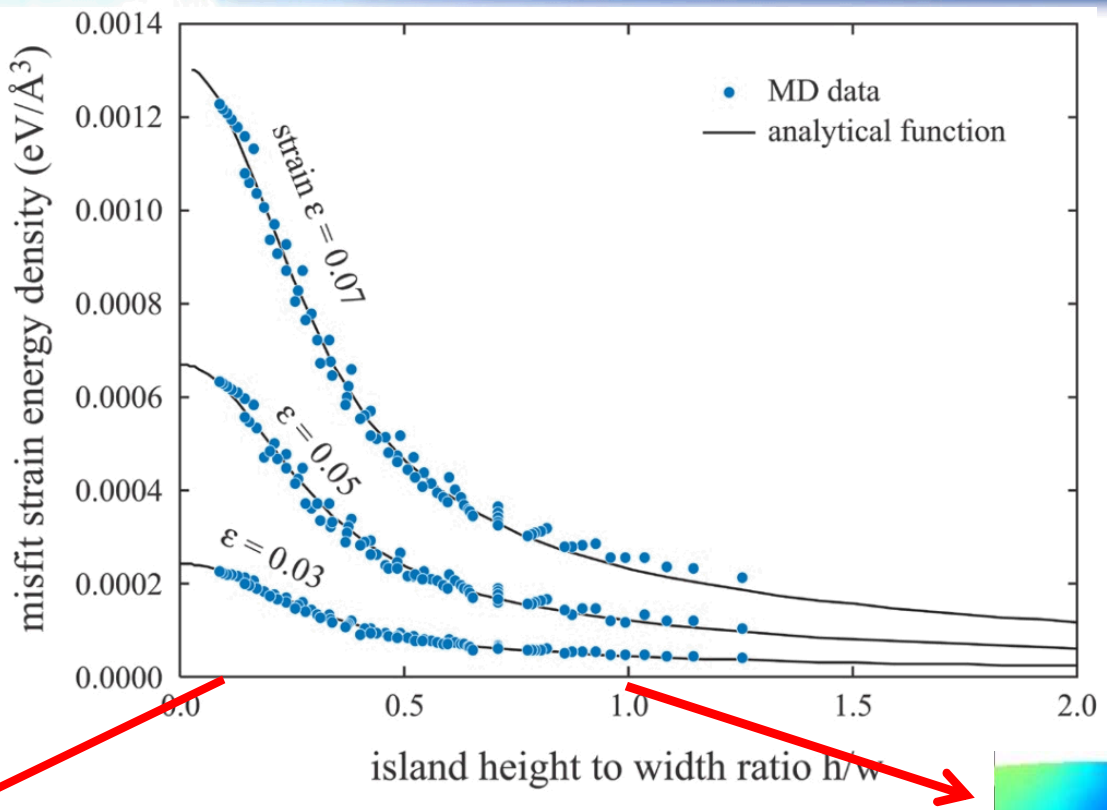


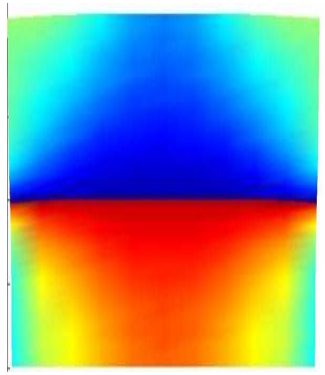
BOP has calculated CdxZn1-xTe/CdS critical diameter

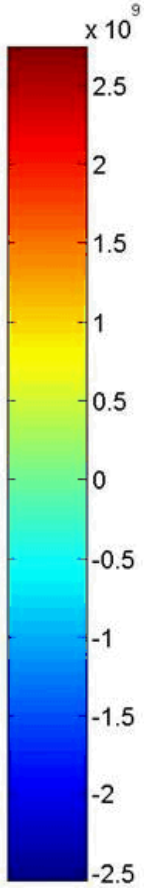


- Critical Island Width, W (fixed substrate)
  - CdTe-CdS: 4 nm
  - ZnTe-CdS: 40 nm
  - ZnTe-CdS: 100 nm (only 5 dislocations)

BOP has calculated critical thickness based on misfit strain and dislocation energy

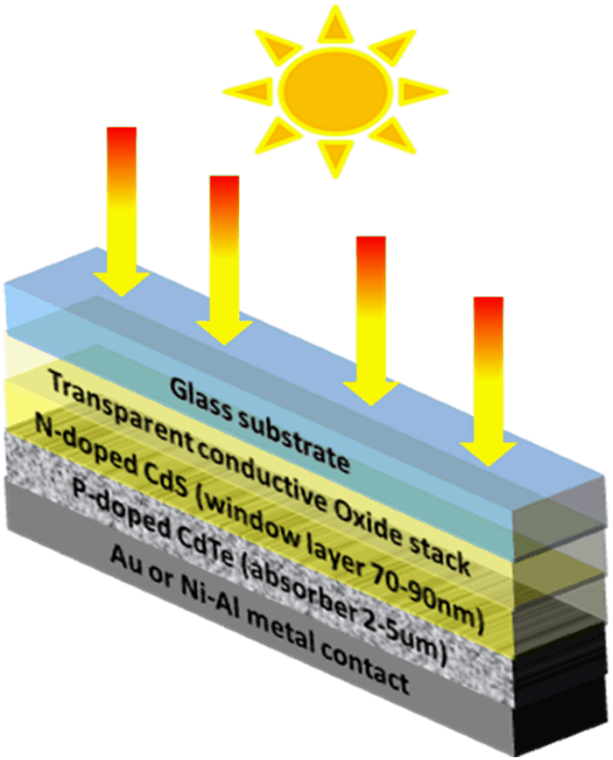


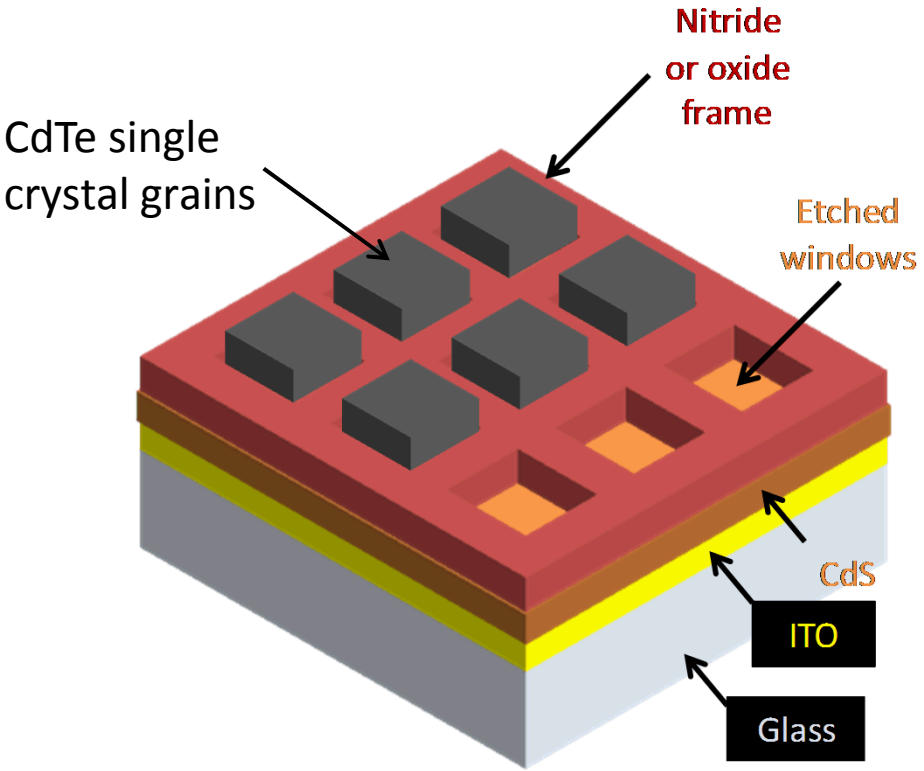




3. Initial Results

We are focusing a on the nanopatterning and the growth of grains



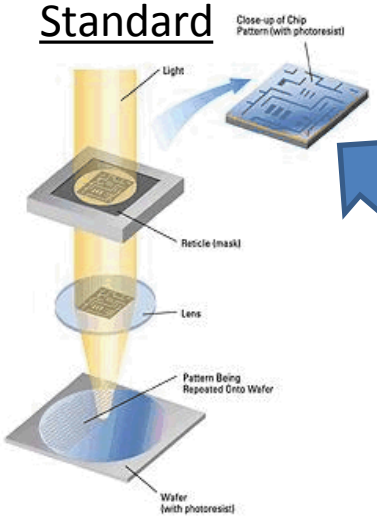


We have tried 4 different lithography techniques to achieve a nanopattern

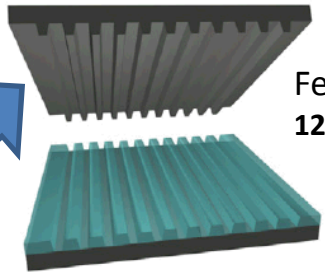
Nanopatterning

Standard

Feature size
200-500nm

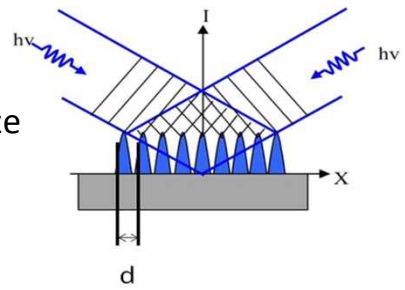


Nano Imprint



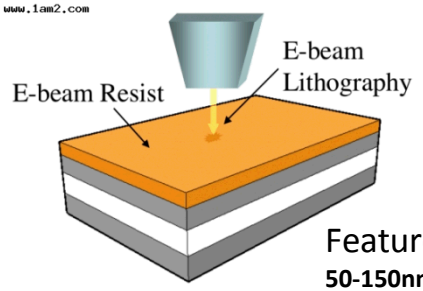
Feature size
125-275nm

Interferometry



Feature size
150-250nm

eBeam



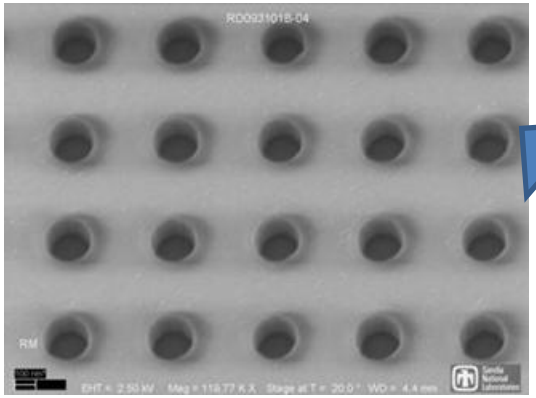
Feature size
50-150nm

[1] P. Carlberg, Development of Nanoimprint Lithography for Applications in Electronics, Photonics and Life-sciences, Doctoral thesis, Dpt. of Phys. Div. of Solid State Phys. Lund University (2006)
[2] F. Zhang, L. Zhang, R. Claus, Investigation of the Photoresist Pattern Profile Contrast Improvement in Interference Lithography Technique Using 488-nm Laser, IEEE Trans. Sem. Manufac., 21 (2008) 464-468

We have tried 4 different lithography techniques to achieve a nanopattern

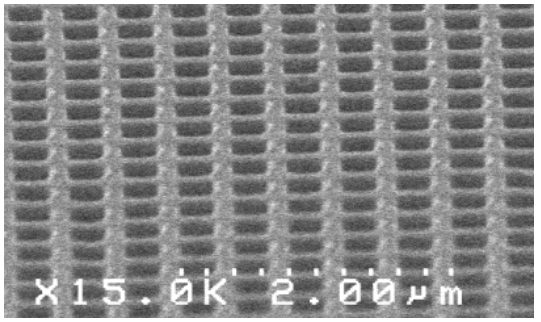
Nanopatterning

Standard



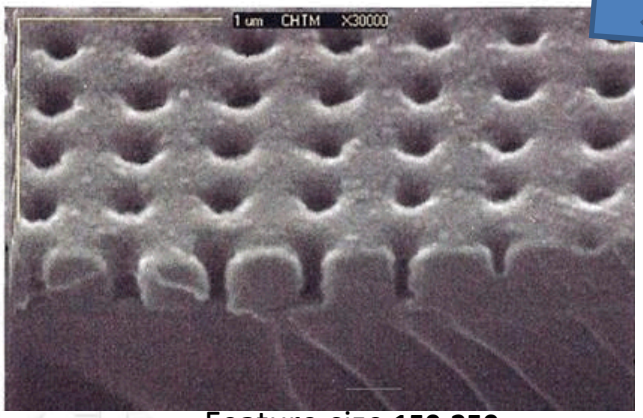
Feature size **200-500nm**

Nano Imprint



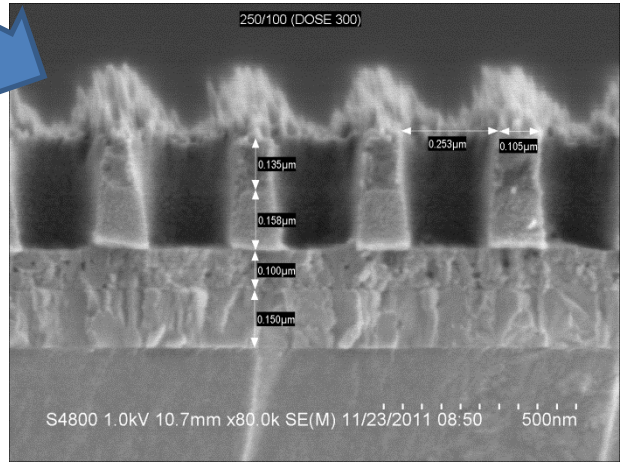
Feature size **125-275nm**

Interferometry



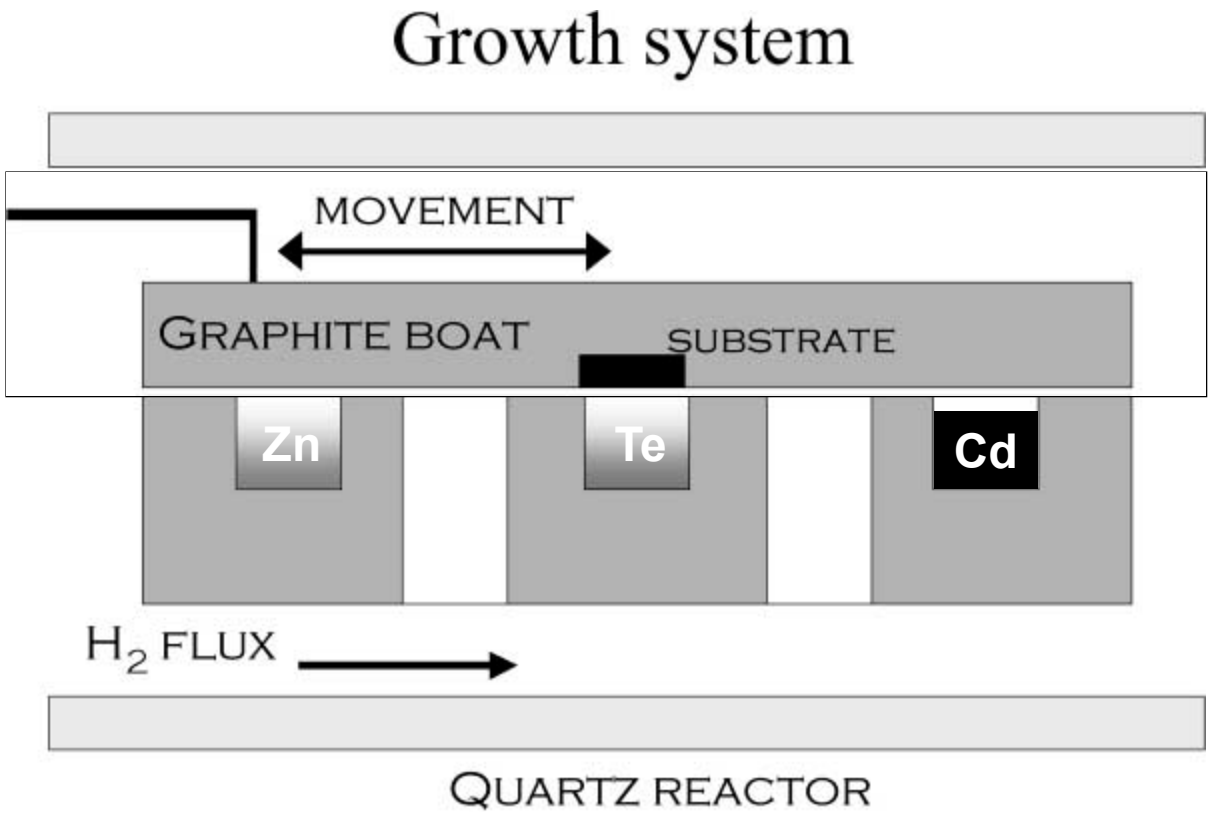
Feature size **150-250nm**

eBeam



Feature size **50-150nm**

ZnCdTe Sublimation Depositor alternates between sources in a linear mode



Pres. = 1 Torr

Temp = 380C

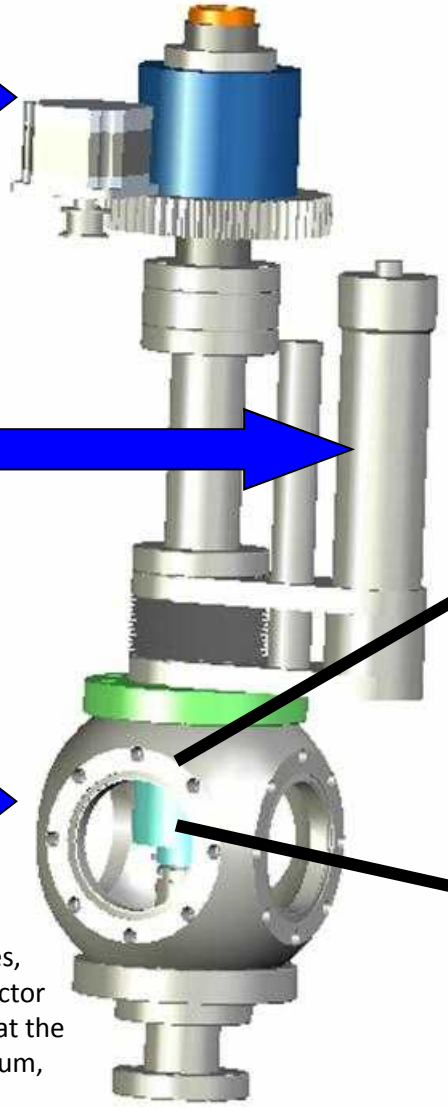
E.M. Larramendi, E. Puron, L.C. Hernandez, M. Sanchez, S. De Roux, O. de Melo, G. Romero-Paredes, R. Pena-Sierra, M. Tamura, "Atomic layer epitaxy of ZnTe by isothermal closed space sublimation," Journal of Crystal Growth 223 (2001) 447–449

UTEP design is a rotary reactor to deposit ZnCdTe from three sources

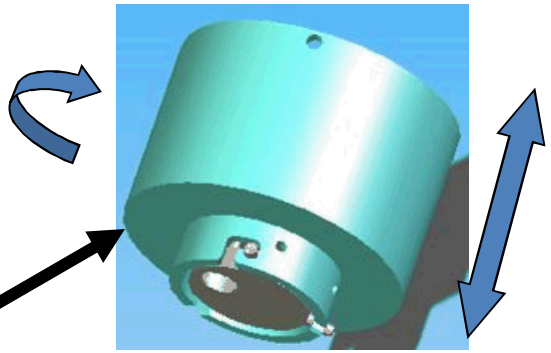
Rotation motor

Source-substrate separation motor

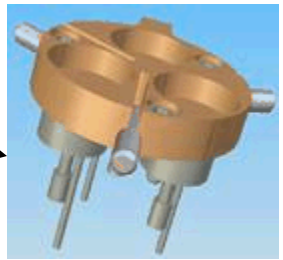
Growth chamber



Off-axis substrate holder
- Rotates
- Moves vertically

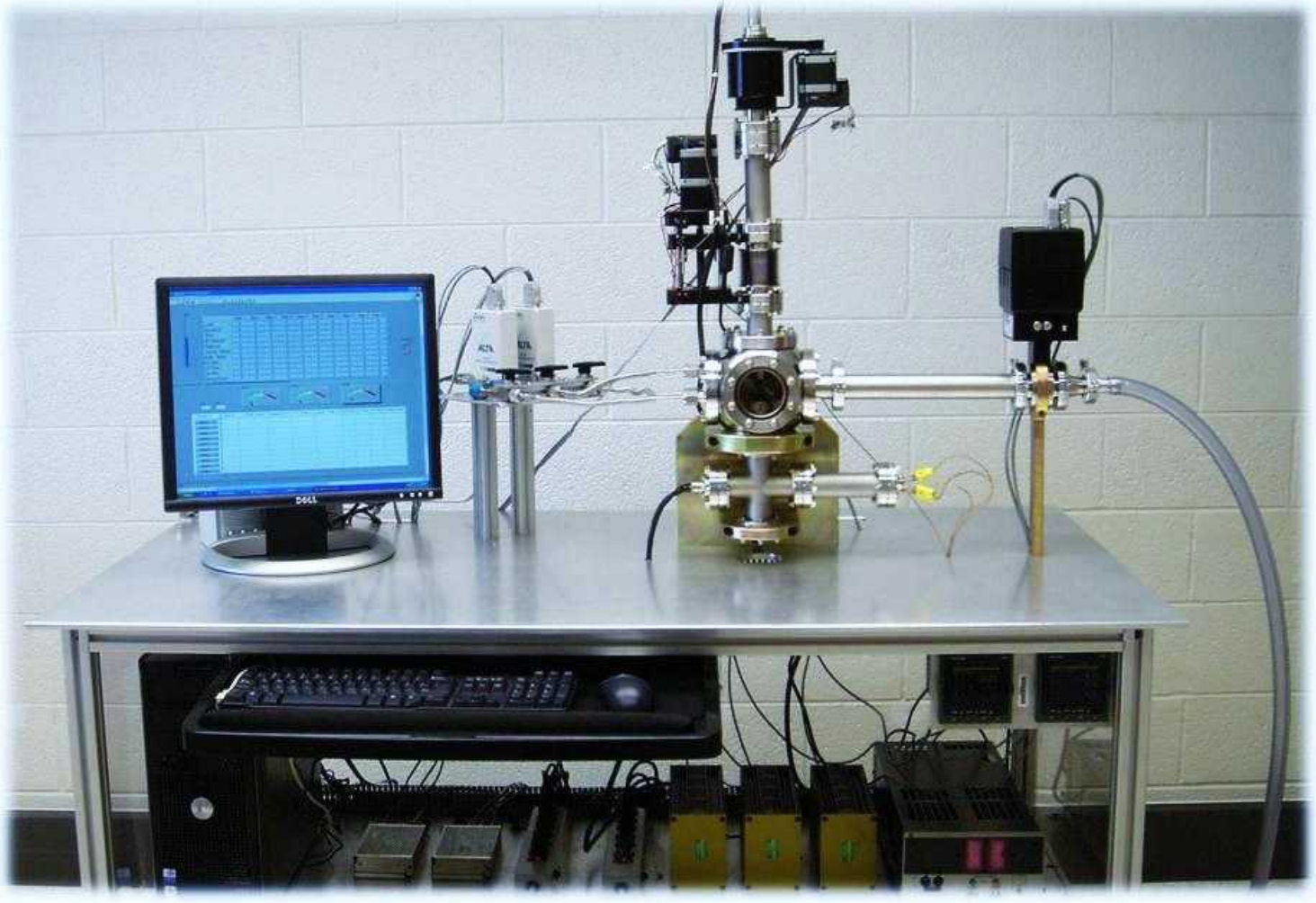


Source holders
- Stationary



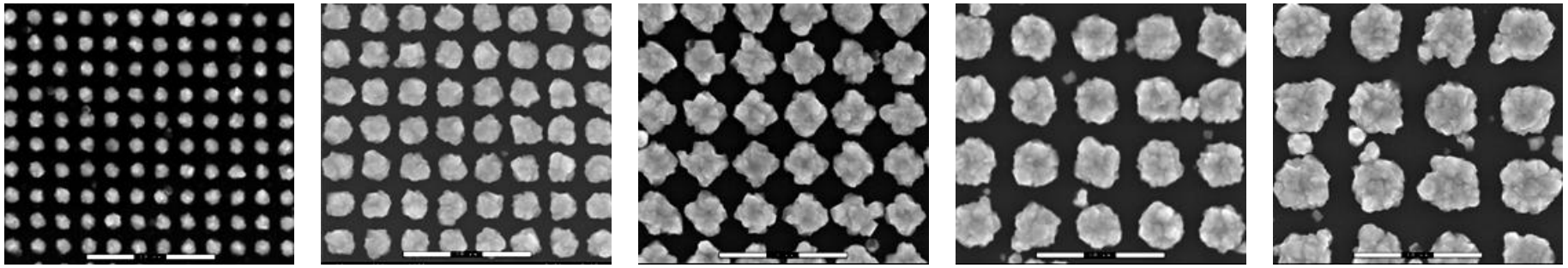
Jacob Rascon, Luis Romo, Scott Rogers, Stella Quinones, John McClure and David Zubia, "New Sublimation Reactor for Epitaxial Growth of II-VI Films", poster, presented at the American Vacuum Society 53rd International Symposium, San Francisco, California, November 14th, 2006.

ZnCdTe Sublimation Depositor



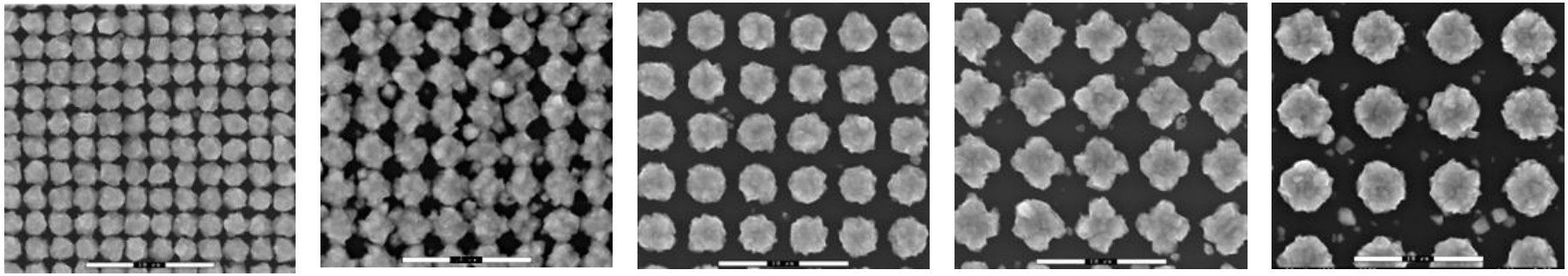
We have achieved selective CdTe deposition on CdS on micron size windows

- 300 nm CdTe



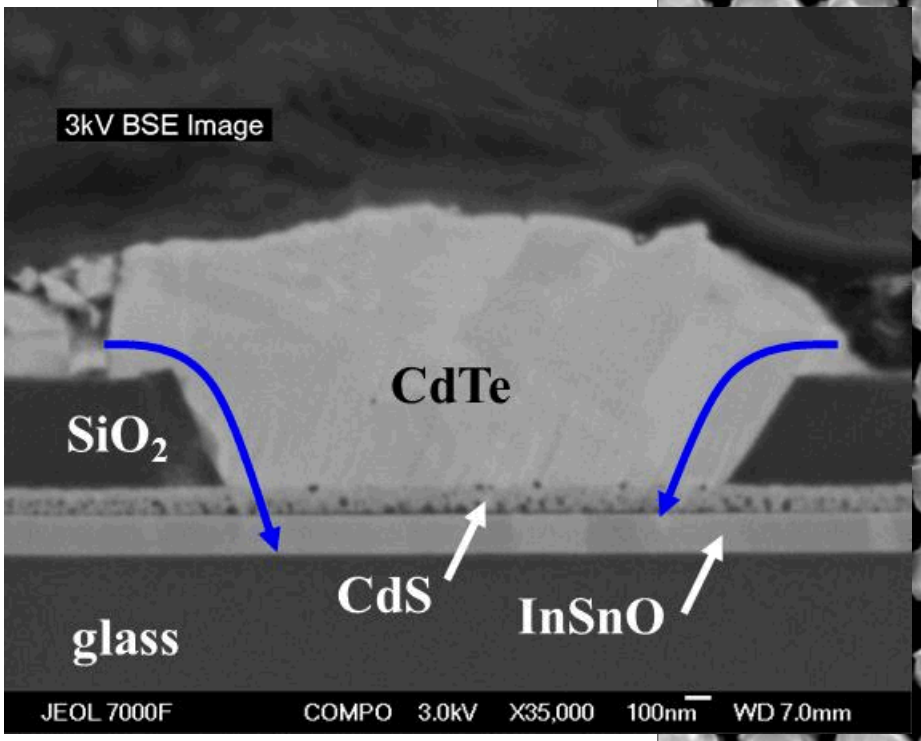
1um 1.5um 2um 2.5um 3um

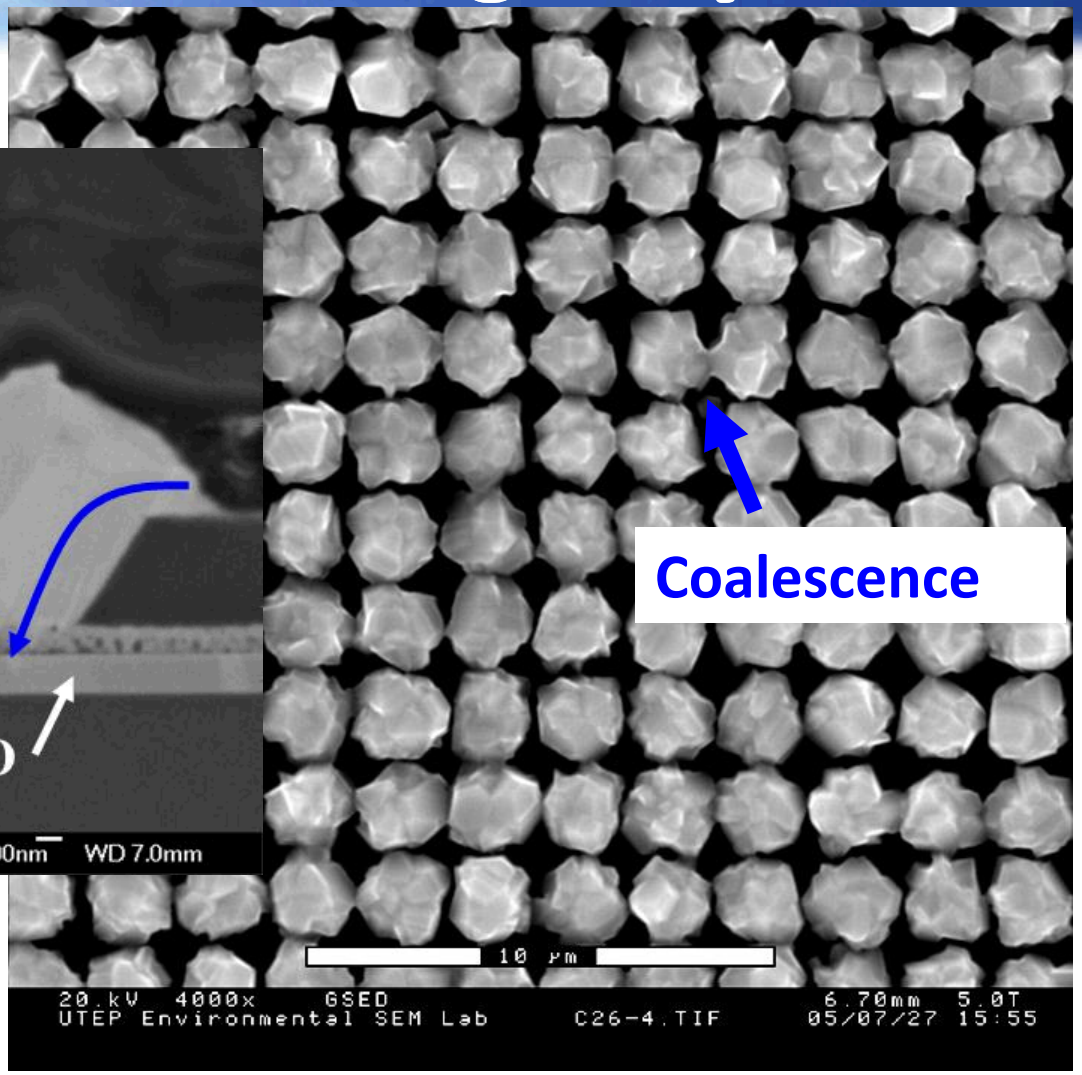
- 750 nm CdTe



David Zubia, Cesar Lopez, Mario Rodrguez, Arev Escobedo, Sandra Oyer, Luis Romo, Scott Rogers, Stella Quinones, and John McClure, "Ordered CdTe/CdS Arrays for High-Performance Solar Cells", Journal of Electronic Materials, Vol. 36, No. 12, p. 1599-1603, 2007.

Reducing the size of window is important to have single crystals





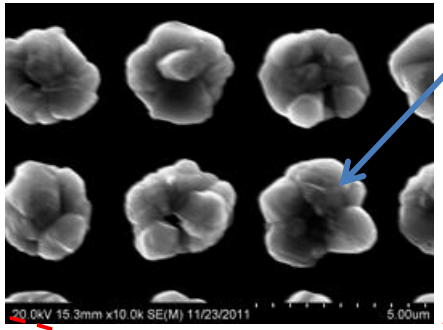
Zubia, David; Romo, Luis; Cruz-Campa, Jose; Aguirre, Brandon; McClure, John; 34th IEEE Photovoltaic Specialists Conference , 2009 , pp: 001842 – 001845
Karpov, V.G., Compaan, A.D., and Shvydka, D. (2002). Effects of nonuniformity in thin-film photovoltaics. *Appl. Phys. Let.* 80, 4256-4258.

Grain size appears to be 100nm in CdTe/SiO2/CdS (2um window) depositions

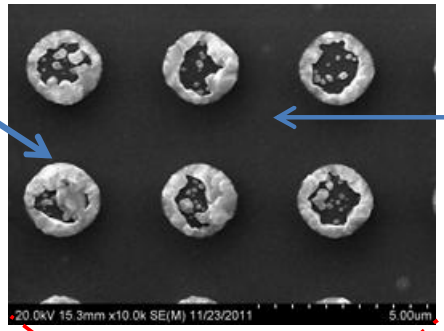
CdTe Selective growth

CdTe nucleation

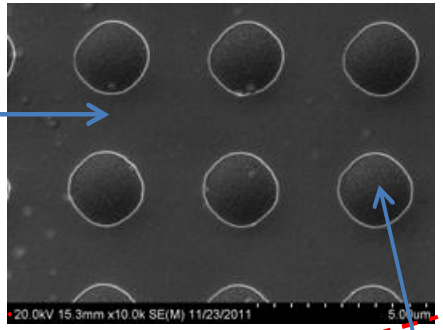
SiO_2 mask on CdS

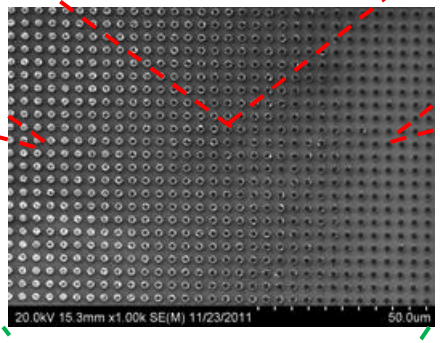


CdTe

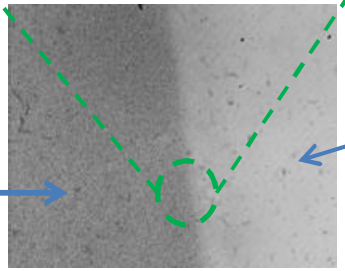


SiO_2





CdS

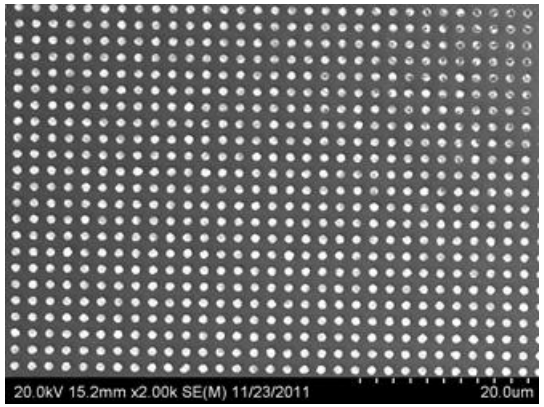


CdTe selective growth on SiO_2/CdS patterned substrates

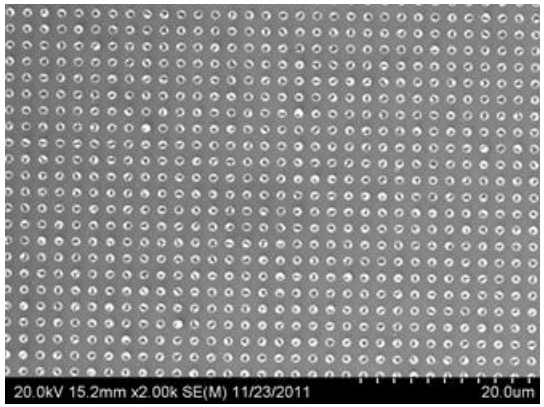
SiO_2/CdS substrate where glass spacer was placed during CdTe deposition

CdTe/SiO2/CdS (1um window)

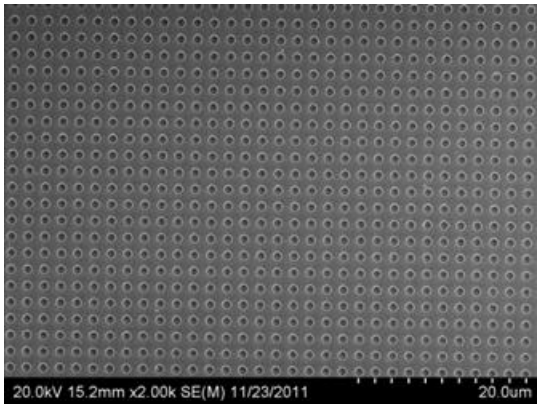
CdTe Selective growth

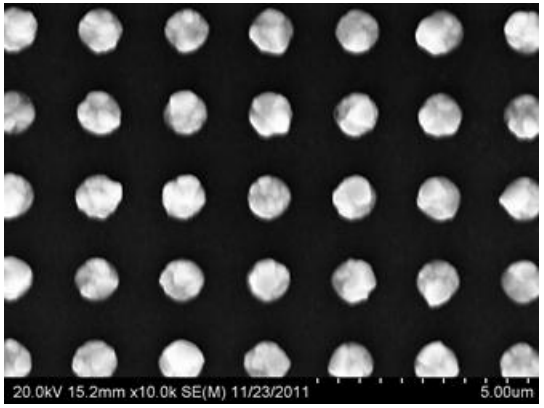


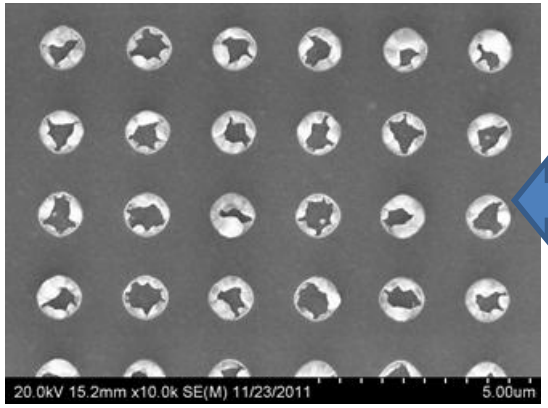
CdTe nucleation



SiO_2 mask on CdS







Higher Magnification of images above

Acknowledgements

- **PI's**
  - David Zubia, Ph.D.
  - Jose Cruz-Campa , Ph.D.
  - Gregory Nielson, Ph.D.
- **Collaborators**
  - Xiaowang Zhou , Ph.D.
  - Jennifer Granata , Ph.D.
  - Erik Spoerke, Ph.D.
  - Bruce Burckel, Ph.D.
  - Calvin Chan, Ph.D.
  - John McClure, Ph.D.
  - Carlos Sanchez
- **Students:**
  - Christian Tapia
  - Jose Chavez
  - Brandon Aguirre
  - Heber Prieto
  - Felipe de Alva
  - Farhana Anwar
  - Damian Marrufo
- **Administrative:**
  - Reagan Stinnett, Ph.D.
  - Michael Kress
  - Alyssa Christy

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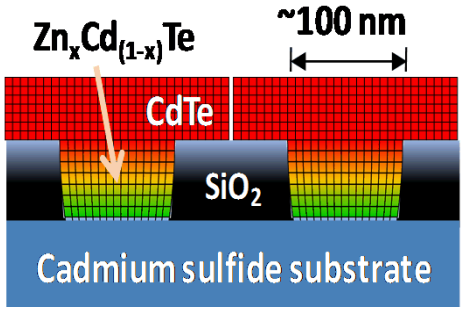
In conclusion we have presented an approach to increase efficiency of CdTe cells



Nanopatterning

Lattice matching

Graded Bandgap

1. Non-uniformity

2. Defects

Current funneling

Light trapping

2. Defects

3. Increase current

4. Better contact

High efficiencies

Questions?