Adhesion and Thermo-Mechanical Reliability in Emerging Thin-Film Device and Energy Technologies

Organosilicate Films

Mark Oliver, Taek-Soo Kim, Yusuke Matsuda, Scott Isaacson

Polymers and Hybrid Nanomaterials

Jeffery Yang, Ruiliang Jia, Marta Giachino, Chaohui Wang, Linying Cui

Ultra-Thin Barrier Films

Ryan Birringer and Tissa Mirfakhrai

Chip Package Interactions

Alex Hsing and Ryan Brock

Photovoltaic and Flexible Electronic Materials

Fernando Novoa, Chris Bruner, Stephanie Dupont, Warren Cui

Biological Hybrids

Krysta Biniek, Olgaby Martinez, Mai Bui, Kemal Levi

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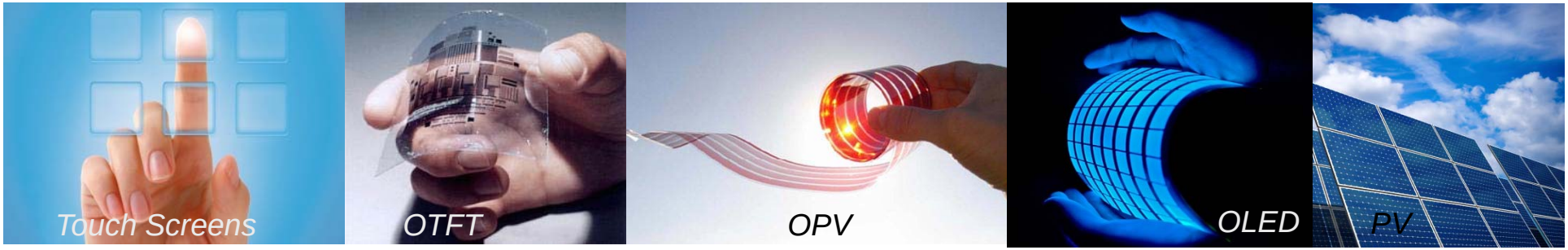
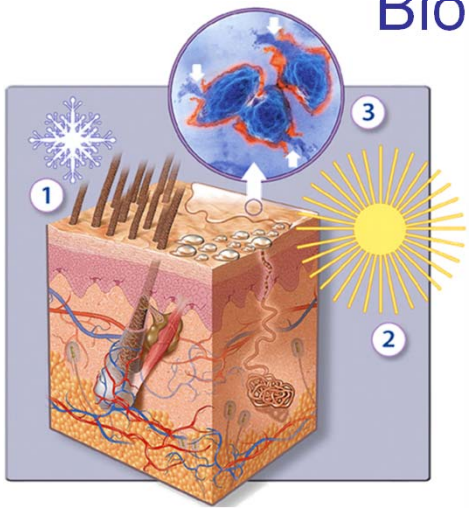
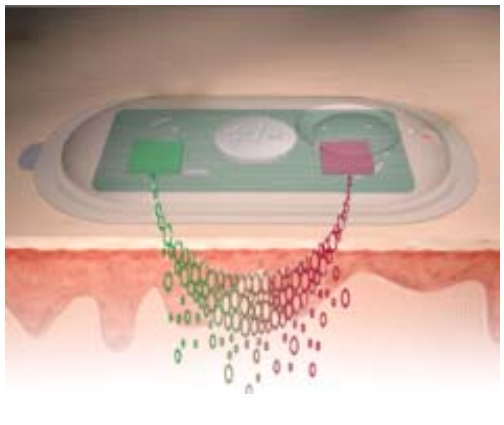
Molecular Hybrid Films in Device Technologies



Bioscience

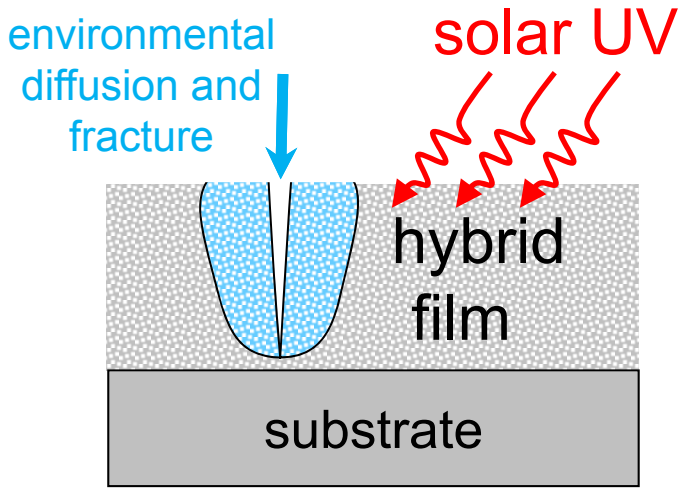


skin science



sensing and drug delivery

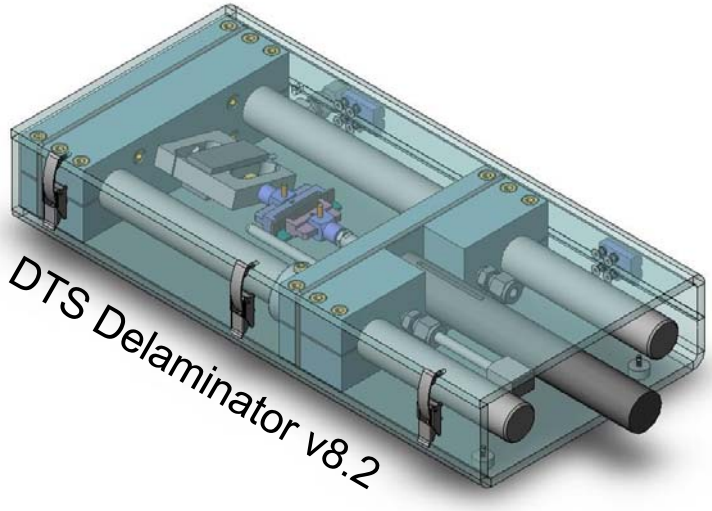
…but hybrid films can be fragile and exposed to harsh environments!

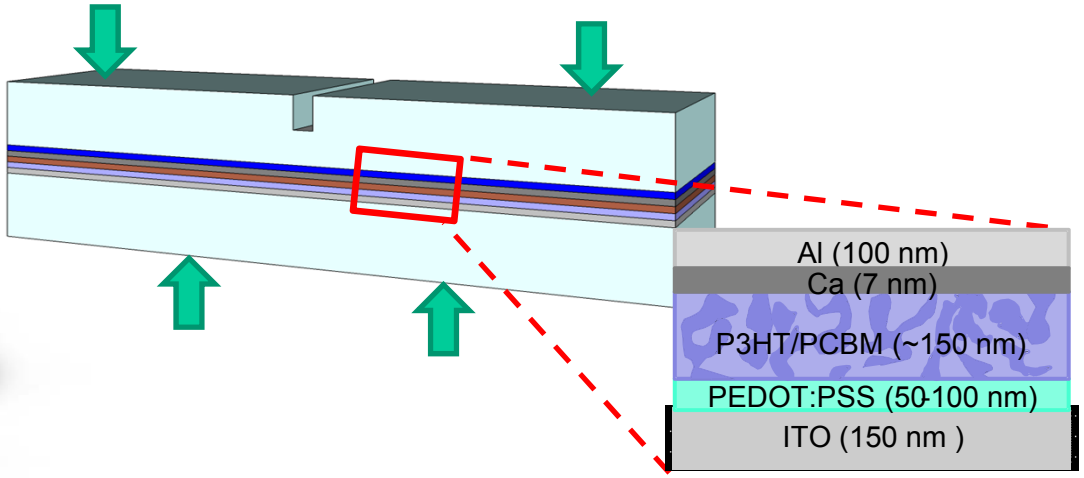


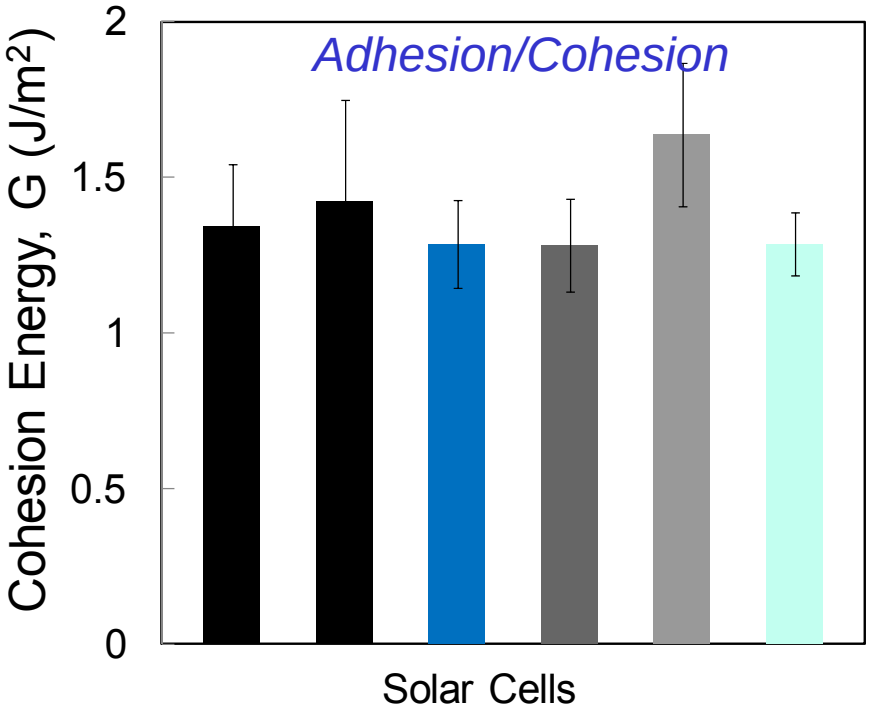
Outline

- Molecular Modeling and Design of Hybrids
  - molecular structure and mechanical properties
- High-Toughness Ceramic-Like SiC:H Films
  - toughening devices with plastic a-SiC:H layers
- Hybrid Materials in Plastic Electronics and OPV
  - cohesion and adhesion, kinetics and lifetimes
- Biological Hybrid Films and Treatments
  - biomechanics of human skin, UV exposure and treatment

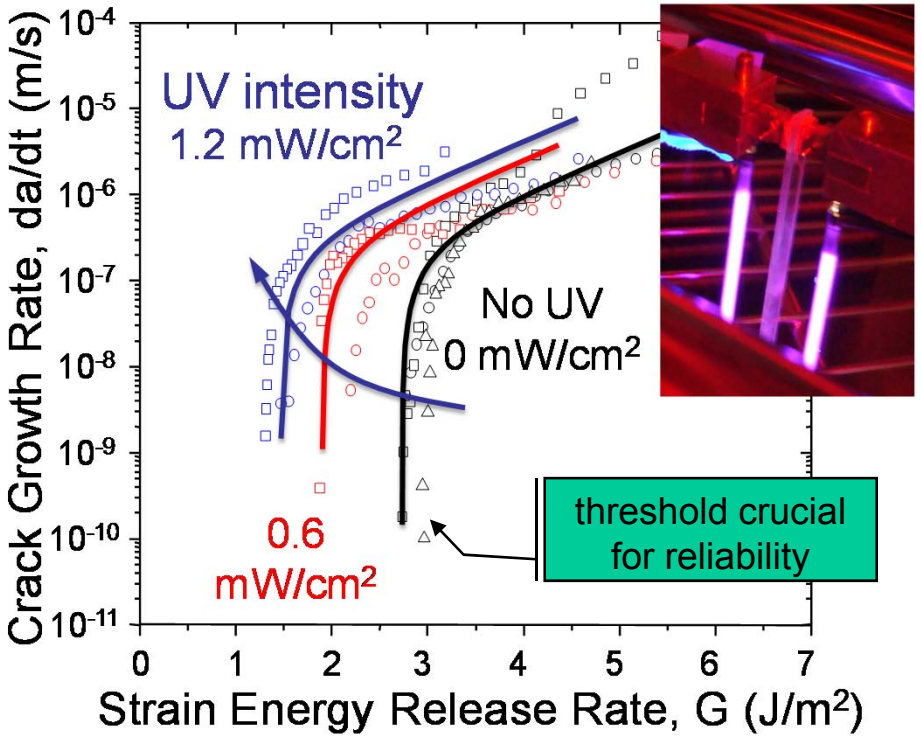
Quantitative Adhesion/Cohesion and Debond Kinetics





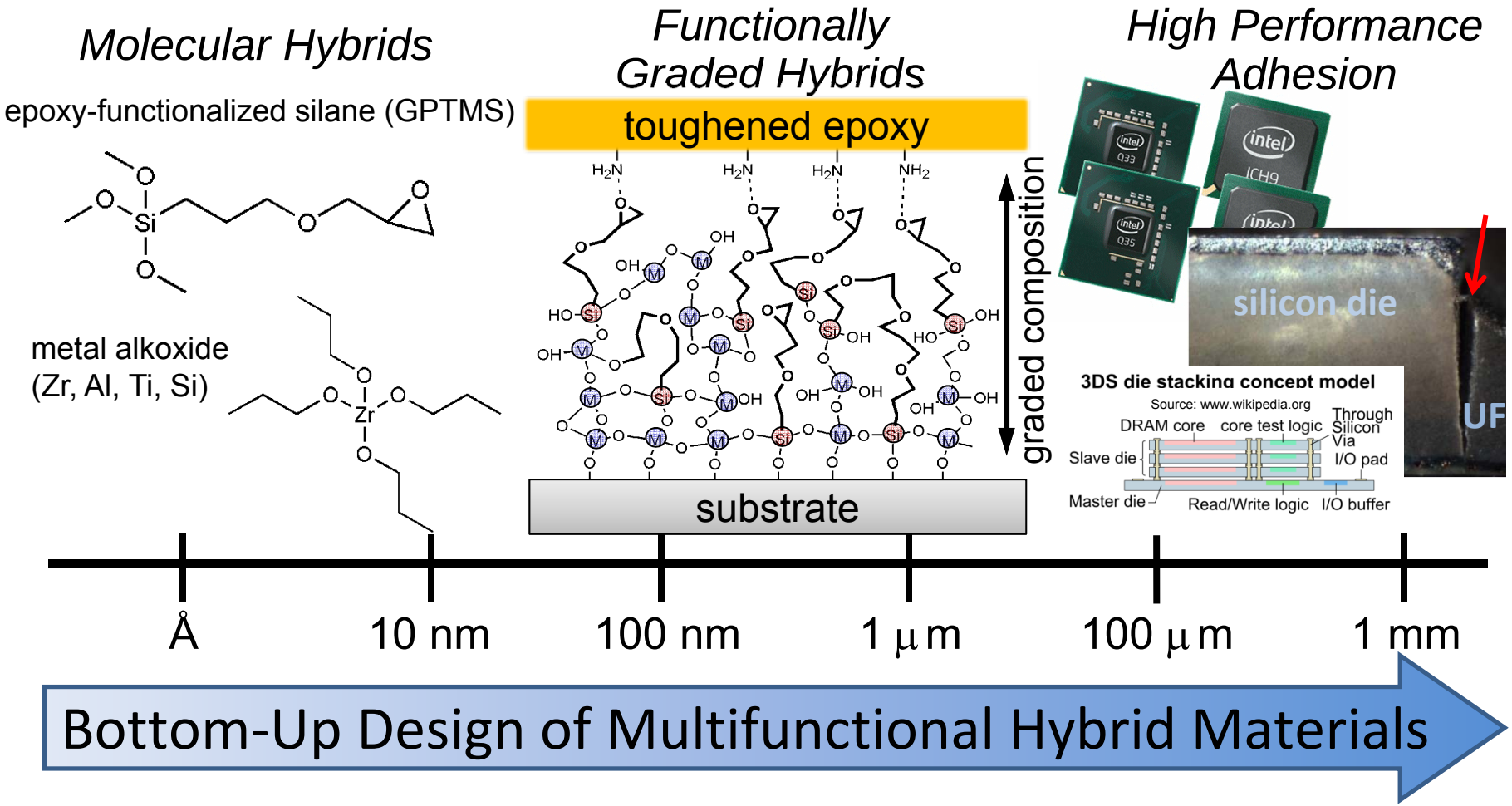


Degradation Kinetics (temp/environment /UV effects)



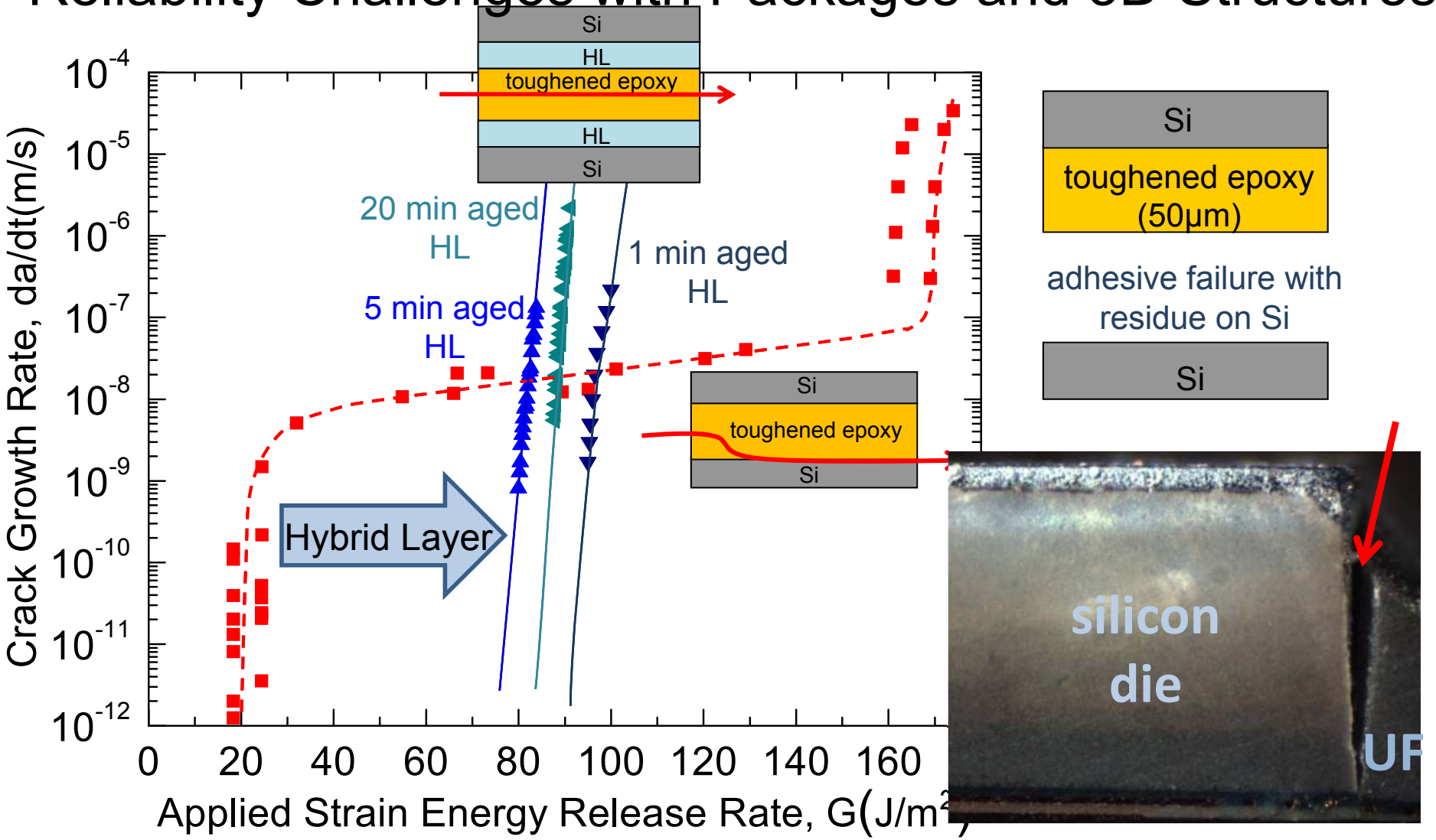
Functionally-Graded Hybrid Layers for High-Performance Adhesion

- *combination of organic and inorganic components from molecular to macro length scales enables materials with multifunctional property sets*
- *opportunity to tailor mechanical, thermal, electrical, and optical properties*



Bottom-Up Design of Multifunctional Hybrid Materials

Reliability Challenges with Packages and 3D Structures



…environmental degradation of toughened UF epoxy, causing continued growth of interfacial defects even at very low loads

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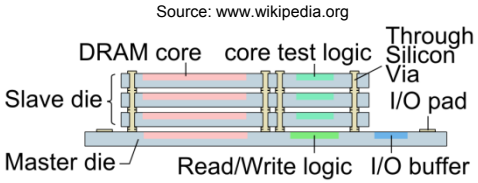
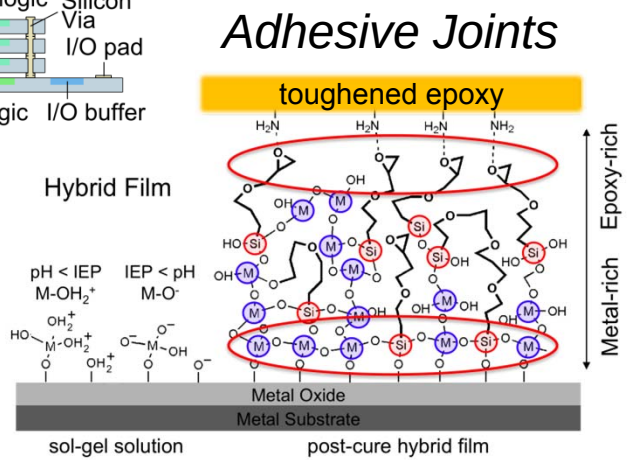
Hybrid Layers for High-Performance Adhesion

Performance Bonding

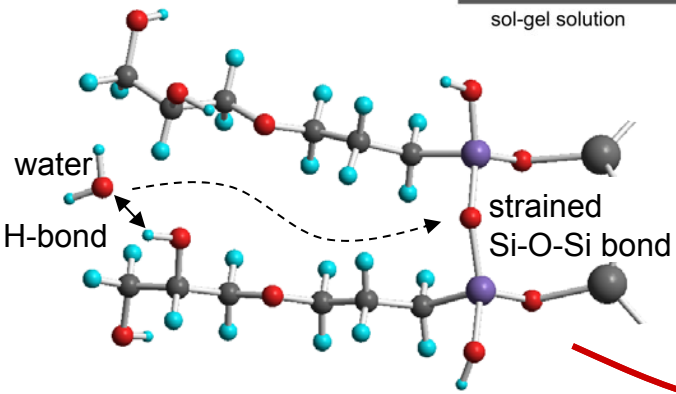
- multiple substrates, 3D structures, embedded sensors, …
- hybrid layer optimization
- single-step dual bonding/barrier layer

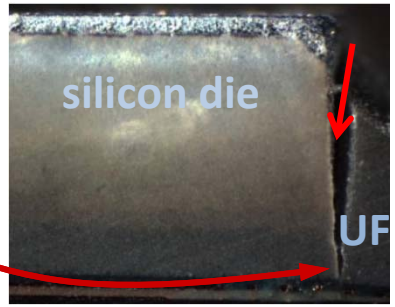




Debonding and Fracture

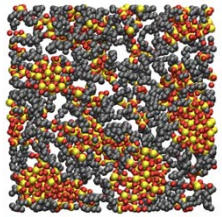
- moisture, temperature and fatigue
- kinetic mechanisms and long-term reliability

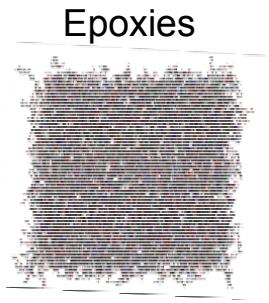




Computational Modeling

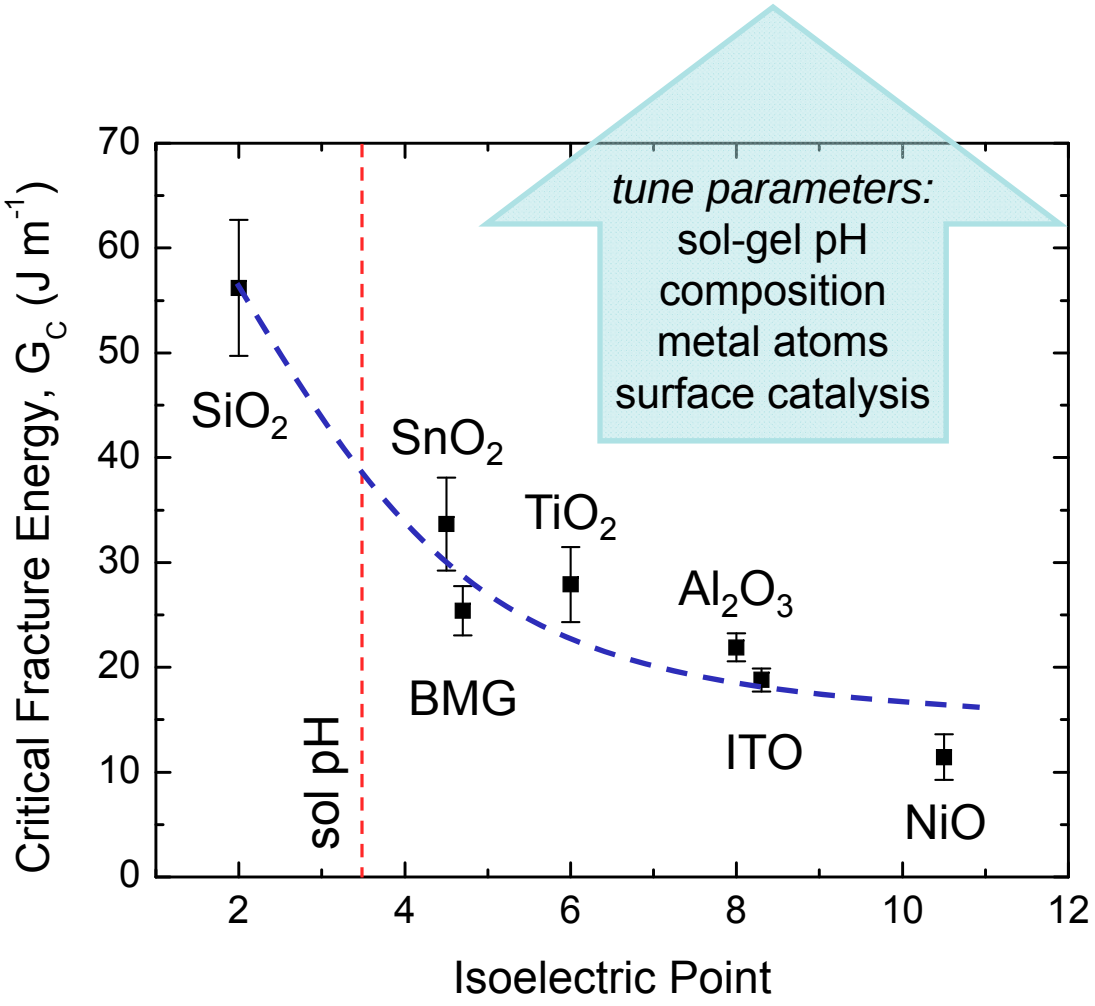
- molecular structure and properties
- new materials discovery





properties
- deformation
- fracture
- fatigue…

Hybrid Layers for High-Performance Adhesion



Substrate	IEP	Max Gc (J/m^2)
WO_3	0.2-0.5	---
SiO_2	1.7-3.5	57.4 ± 7.4
SnO_2	4.5-5	33.6 ± 4.4
BMG	4.7	25.4 ± 2.4
TiO_2	6	27.9 ± 3.6
Al_2O_3	7-8	21.9 ± 1.3
ITO	8.3	18.8 ± 1.1
NiO	10-11	11.4 ± 2.2

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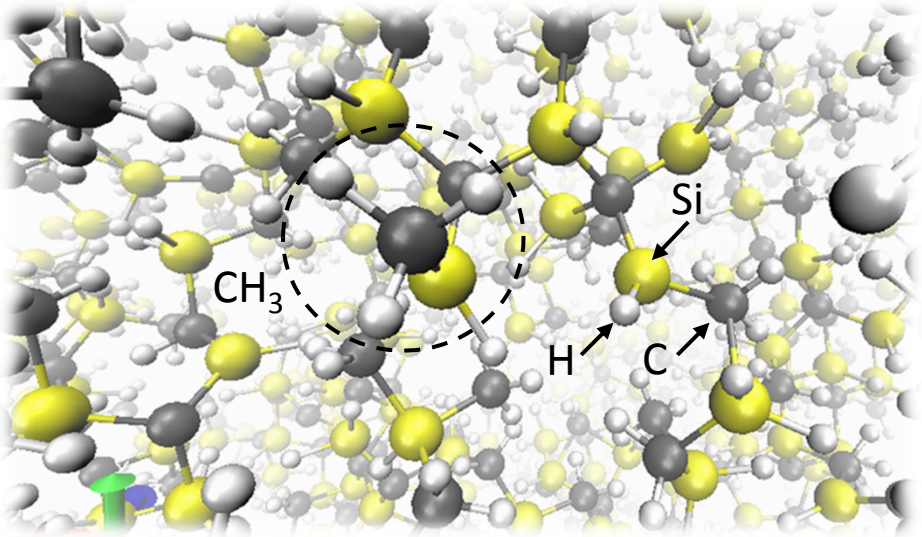
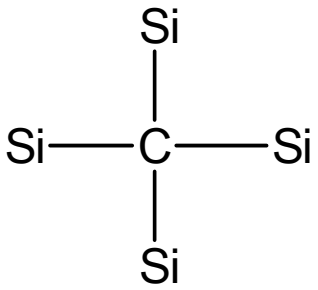
Hydrogenated Amorphous Silicon Carbide (a-SiC:H)

network backbone: Si-C, C=C
terminal groups: -H, -CH_3

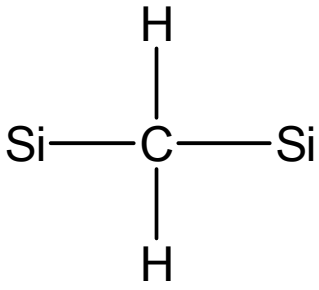


crystalline SiC



fully connected

a-SiC:H



reduced connectivity

- chemical and thermal stability
- unique opt-electrical properties

Si-O-Si bond free…

- low sensitivity to moisture cracking
- can exhibit high fracture resistance

PE-CVD at 400°C

precursors: methylsilane, phenylsilane, He, H_2

stoichiometric (C/Si ~ 1)

non-stoichiometric (C/Si ~ 5)

phenyl organic porogen

Matsuda, King , Dauskardt, Acta Mat. 2011.

Hydrogenated Amorphous Silicon Carbide (a-SiC:H)

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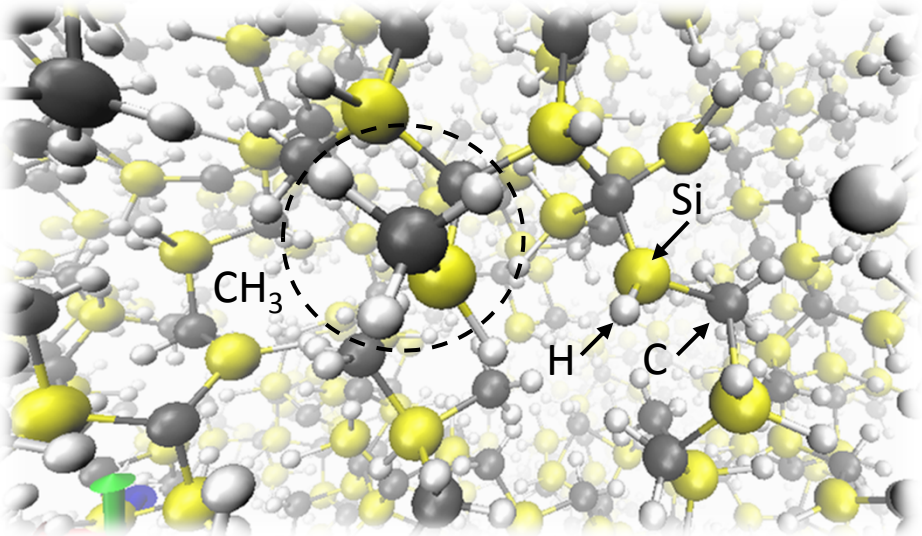
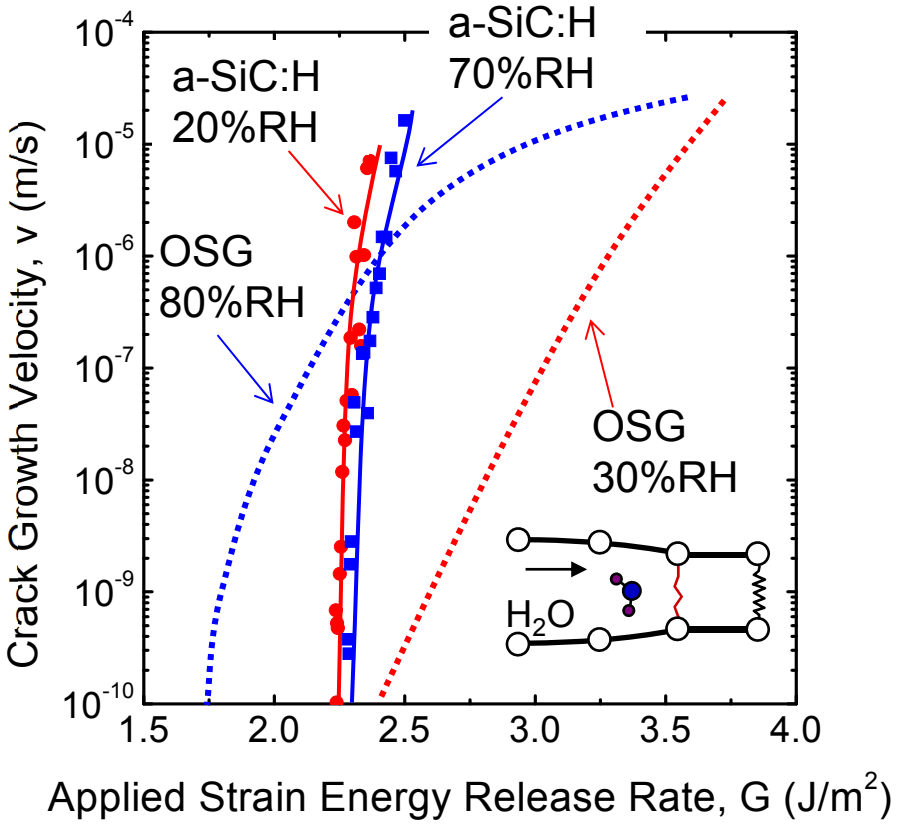


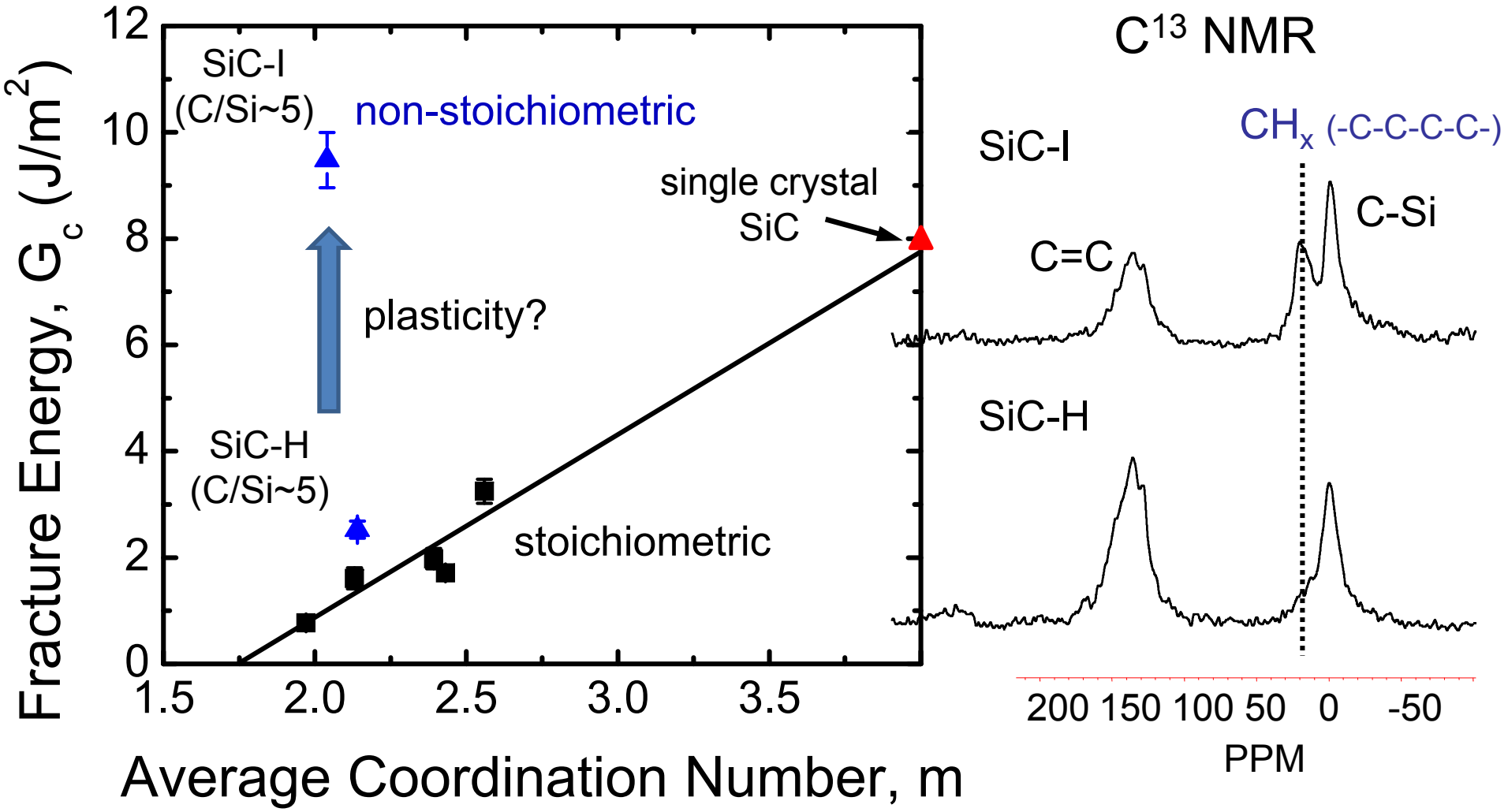


- chemical and thermal stability
- unique opt-electrical properties

Si-O-Si bond free …(trace amounts)
- low sensitivity to moisture cracking
- can exhibit high fracture resistance

Matsuda, King , Dauskardt, Acta Mat. 2011.

Cohesive Fracture Energy and Connectivity



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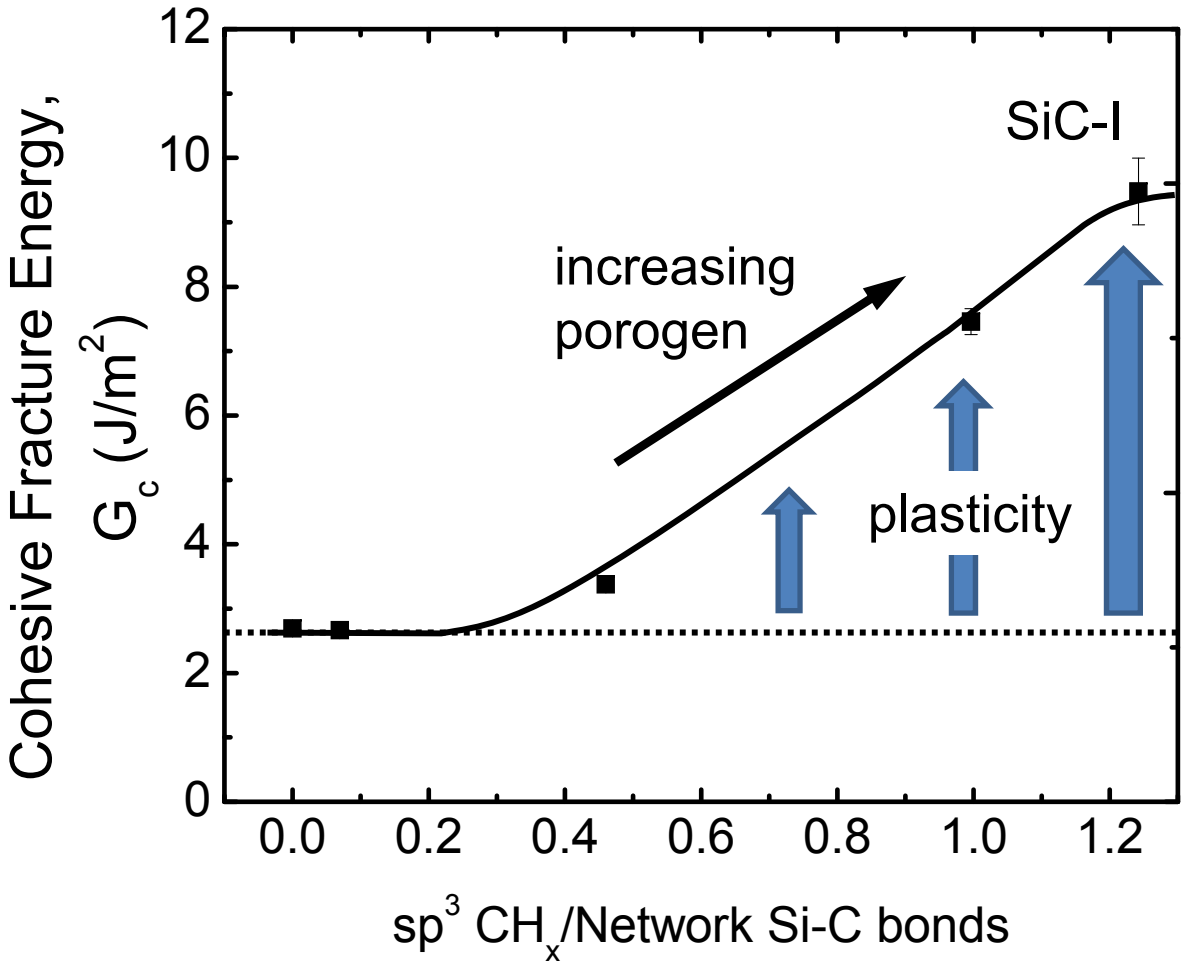
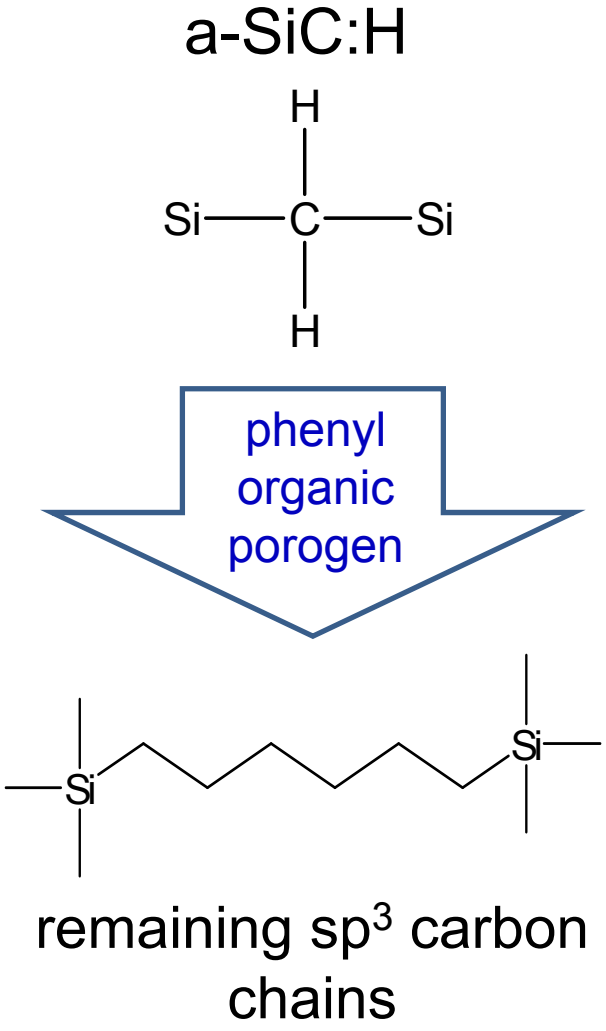
Matsuda, King , Dauskardt, Acta Mat. 2011.

Plasticity in Non-Stoichiometric a-SiC:H Films



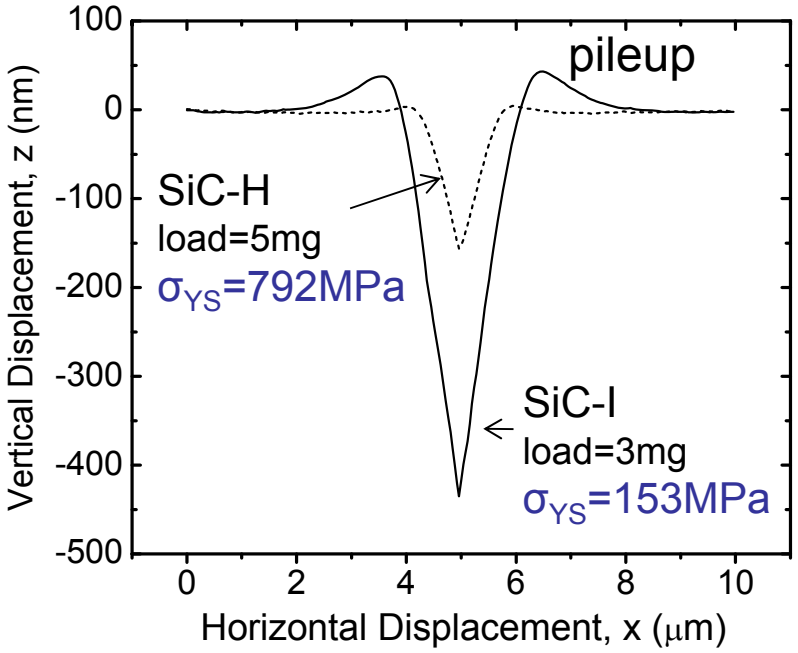


remaining sp^3 carbon chains

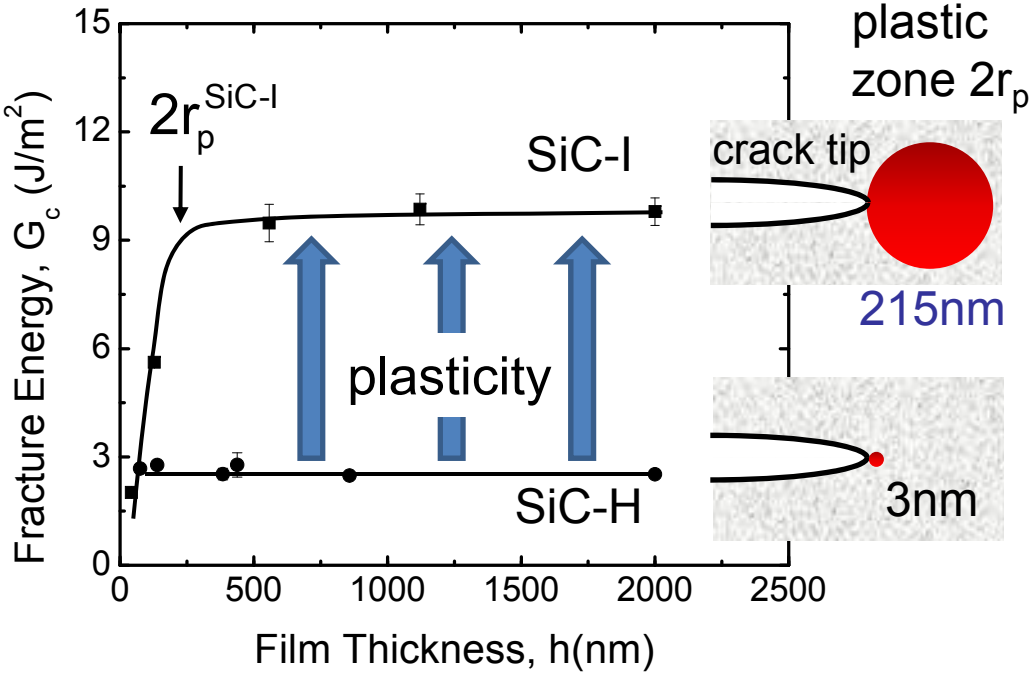
sp^3 CH$_x$/Network Si-C bonds were characterized by FTIR, XRR, and RBS.

Plasticity in Non-Stoichiometric a-SiC:H Films

nanoindentation

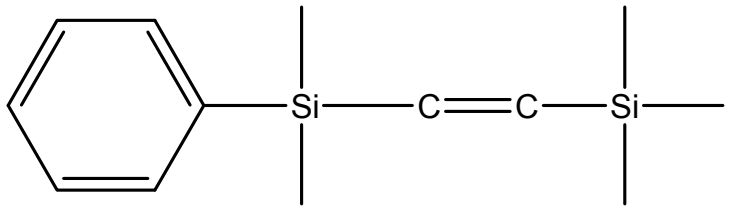


thickness dependence of G_c



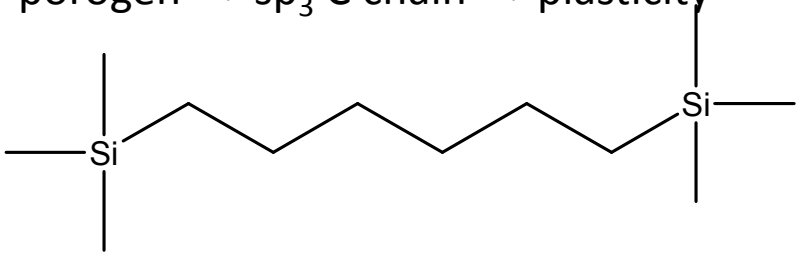
SiC-H (brittle)

phenyl, C=C



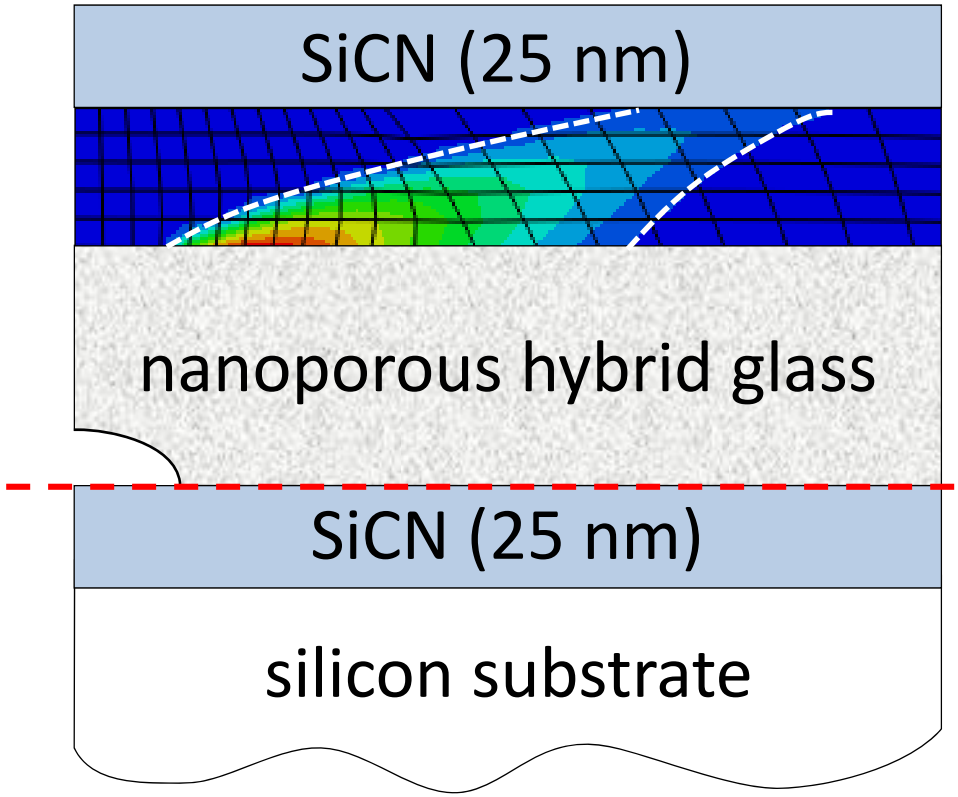
SiC-I (plasticity)

porogen → sp_3 C chain → plasticity

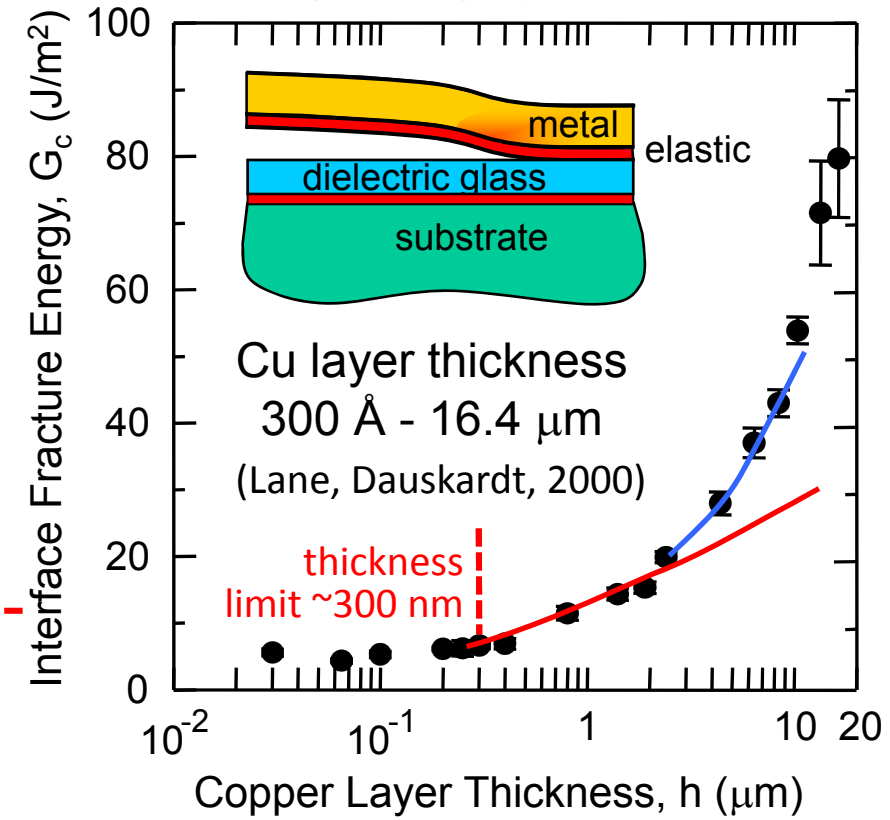


Toughening with Ceramic-Like a-SiC:H Films

$$G_C = G_0 + G_{plasticity}$$



toughening by metal films



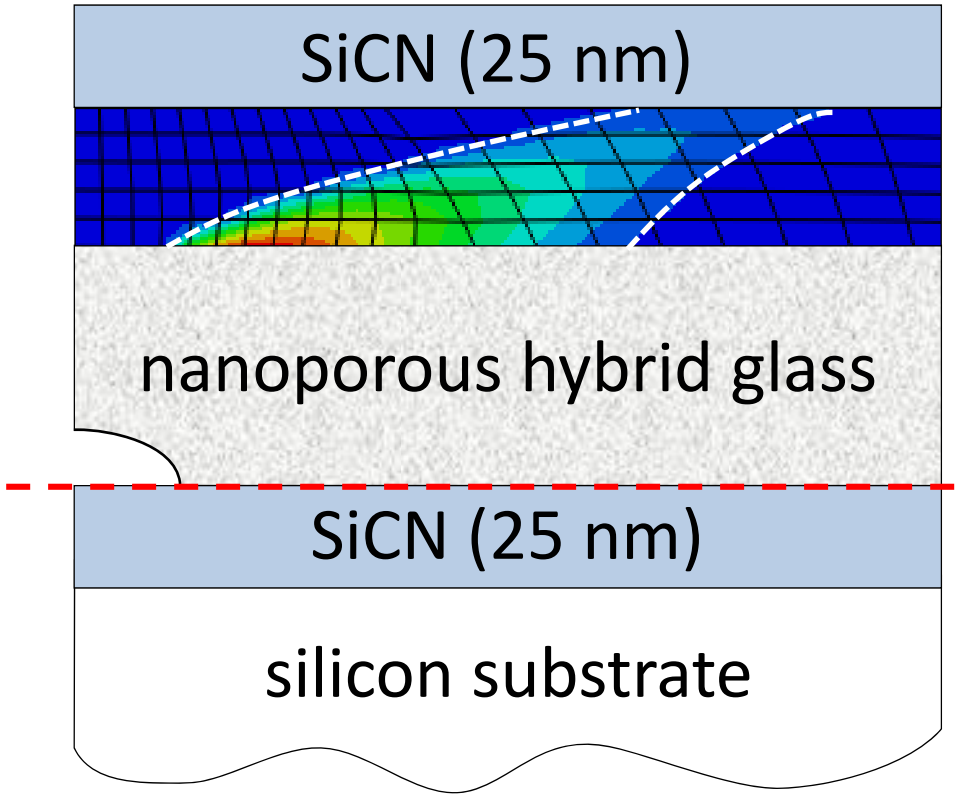
limited metal plasticity at nanoscale

- low dislocation ρ and mobility
- small grain size (Hall-Petch)

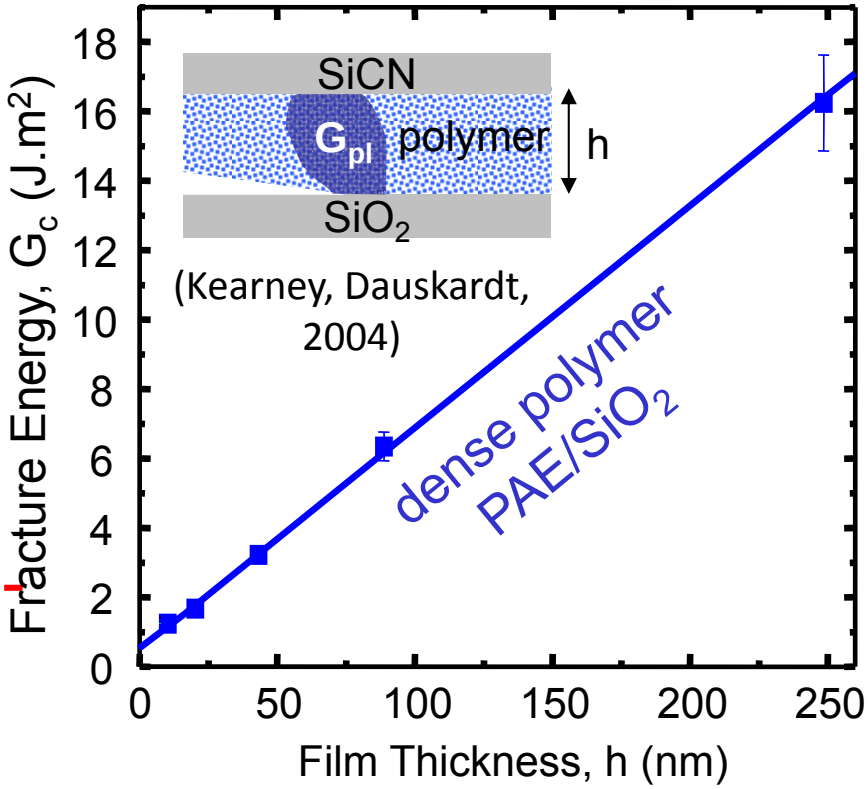
Matsuda, Dauskardt et al., Small, 2012 in review.

Toughening with Ceramic-Like a-SiC:H Films

$$G_C = G_0 + G_{plasticity}$$



toughening by polymer films



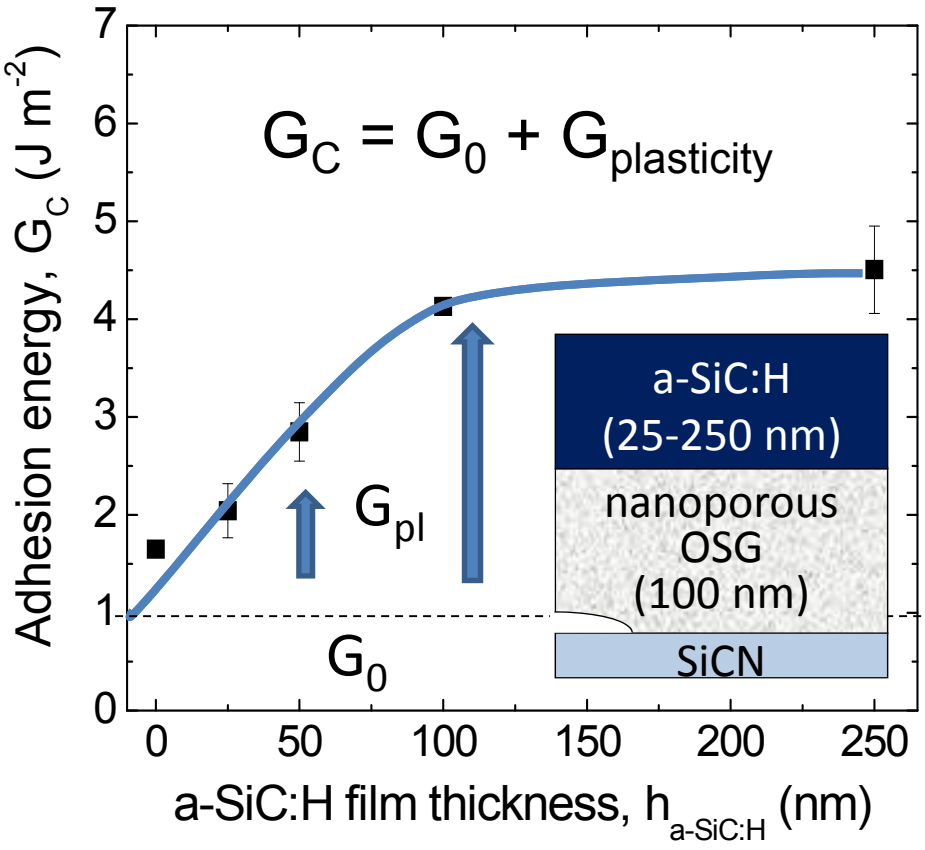
polymer plasticity at nanoscale

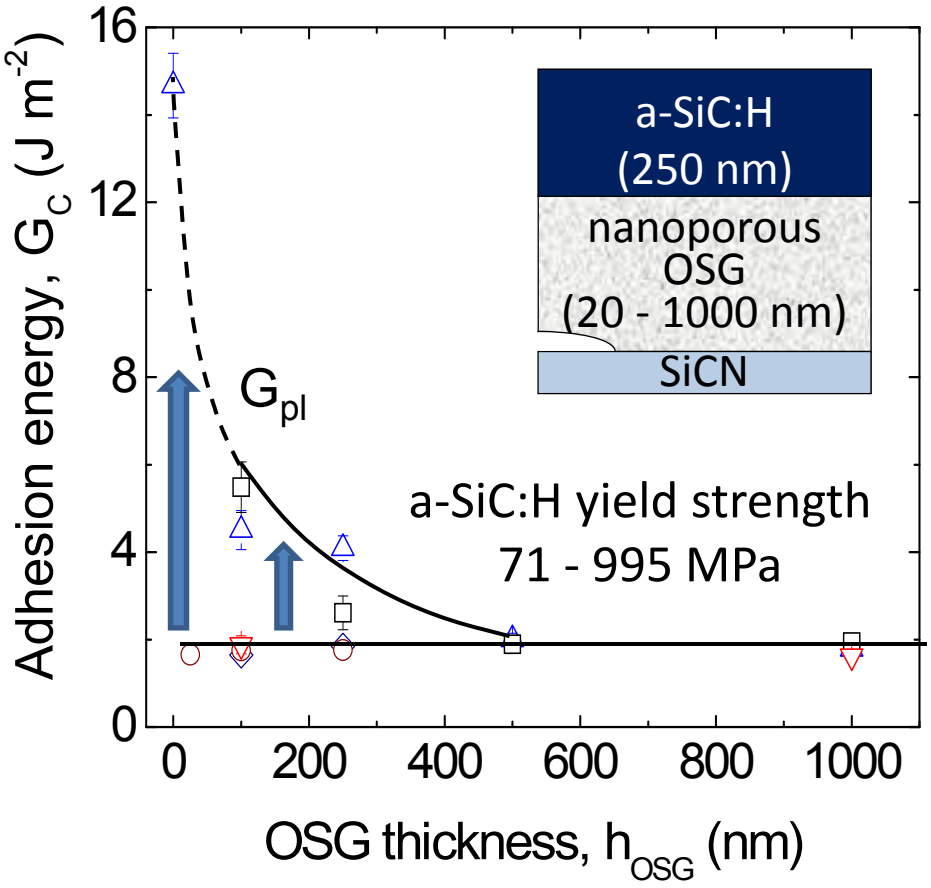
- limited thermal stability
- incompatible deposition

Matsuda, Dauskardt et al., Small, 2012 in review.

Toughening with Ceramic-Like a-SiC:H Films

much more effective toughening than metal films, more thermally stable than polymers





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Matsuda, Dauskardt et al., Small, 2012 in review.

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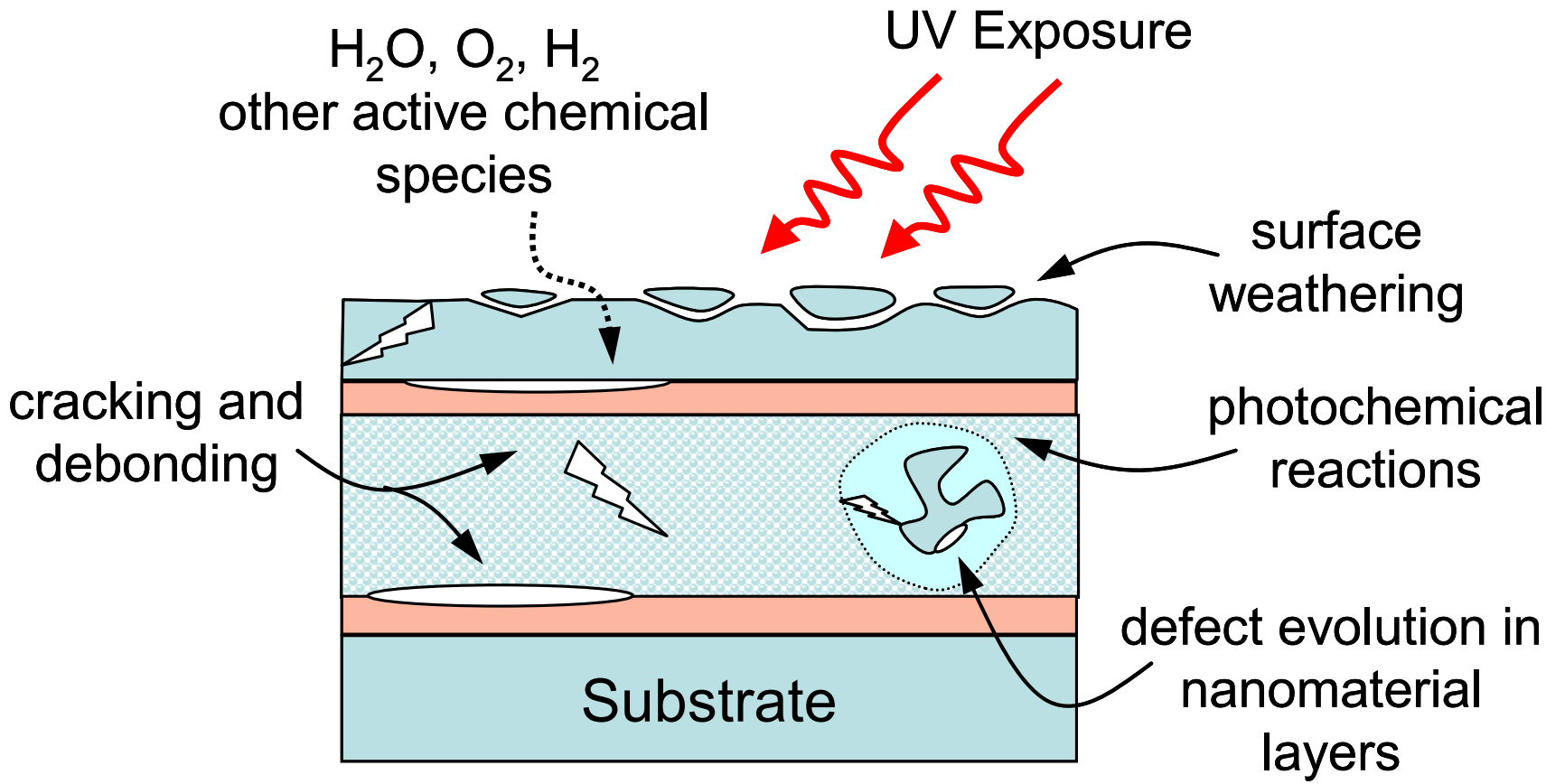
Degradation and Reliability of PV Devices and Modules

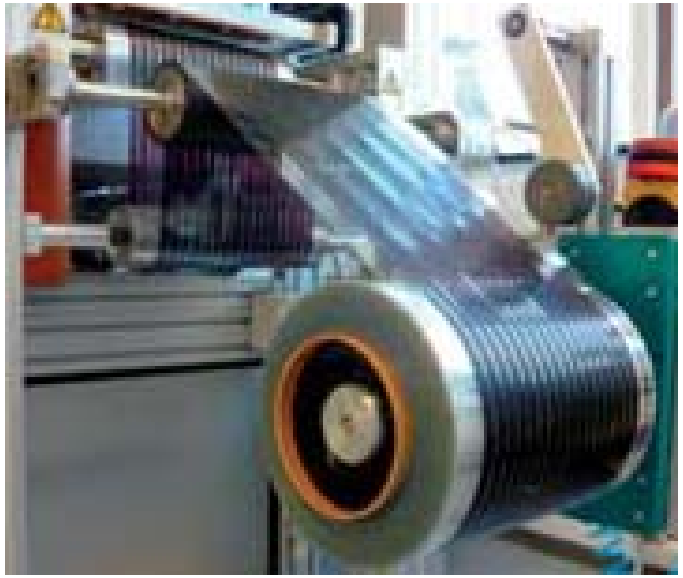


Severe operating environments:

Thermal cycling, mechanical stress, moisture, chemically active environmental species, and solar UV.

Uncertain degradation kinetics and reliability models.

Roll-to-Roll Flexible Inverted Polymer Solar Cell

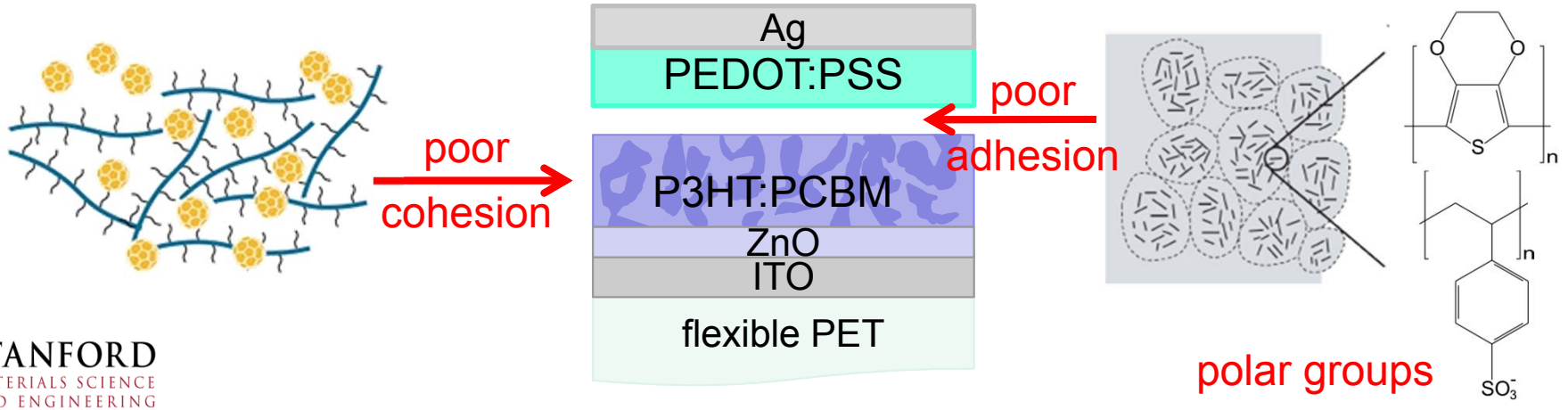


- Manufacturing: automated R2R
  - high throughput
  - large area
- Materials
  - abundant
  - cheap
  - light weight
- Flexible Substrates

Typical Inverted Polymer Solar Cell

P3HT:PCBM → hydrophobic

PEDOT:PSS → hydrophilic



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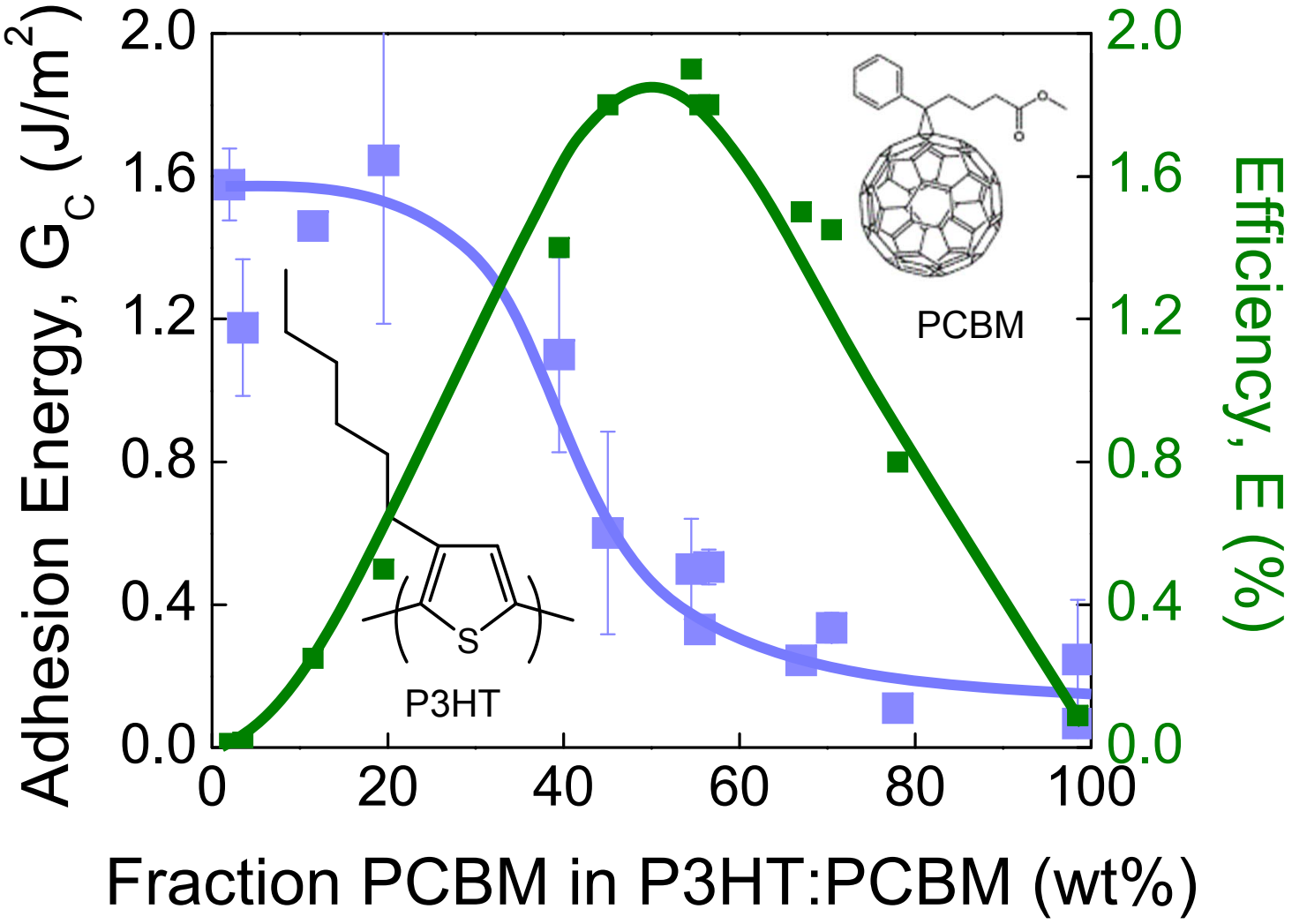
Effect of BHJ Composition on Adhesion



Fullerene rich layers lead to very poor adhesion

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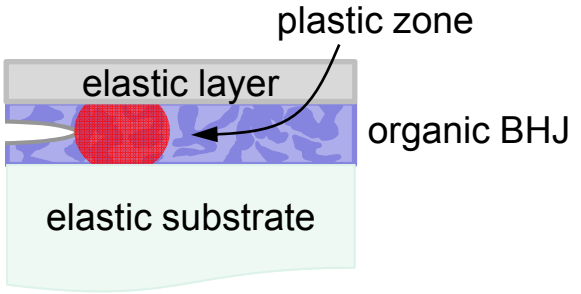
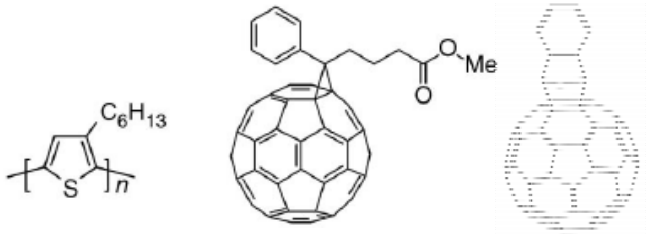
Dupont, Oliver, Krebs, Dauskardt, Sol. Eng. Mat., 2011

Factors Effecting Cohesion of BHJ Layers

- Heterojunction layer thickness
  - is cohesion in organic layers sensitive to layer thickness?

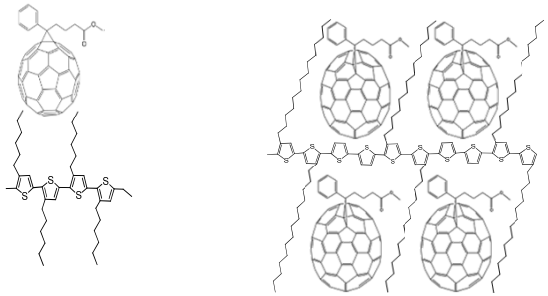


- Composition of the heterojunction layer
  - limited bonding to fullerene
  - polymer/PCBM ratio makes stronger layer

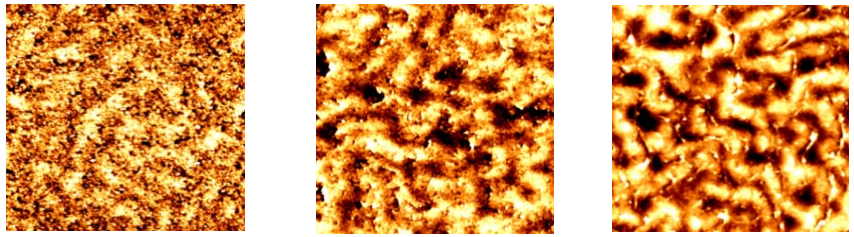


P3HT PCBM Indene C60

- Molecular intercalation
  - manipulating the types of intermolecular interactions



- Annealing
  - morphology of the BHJ layer changes with annealing



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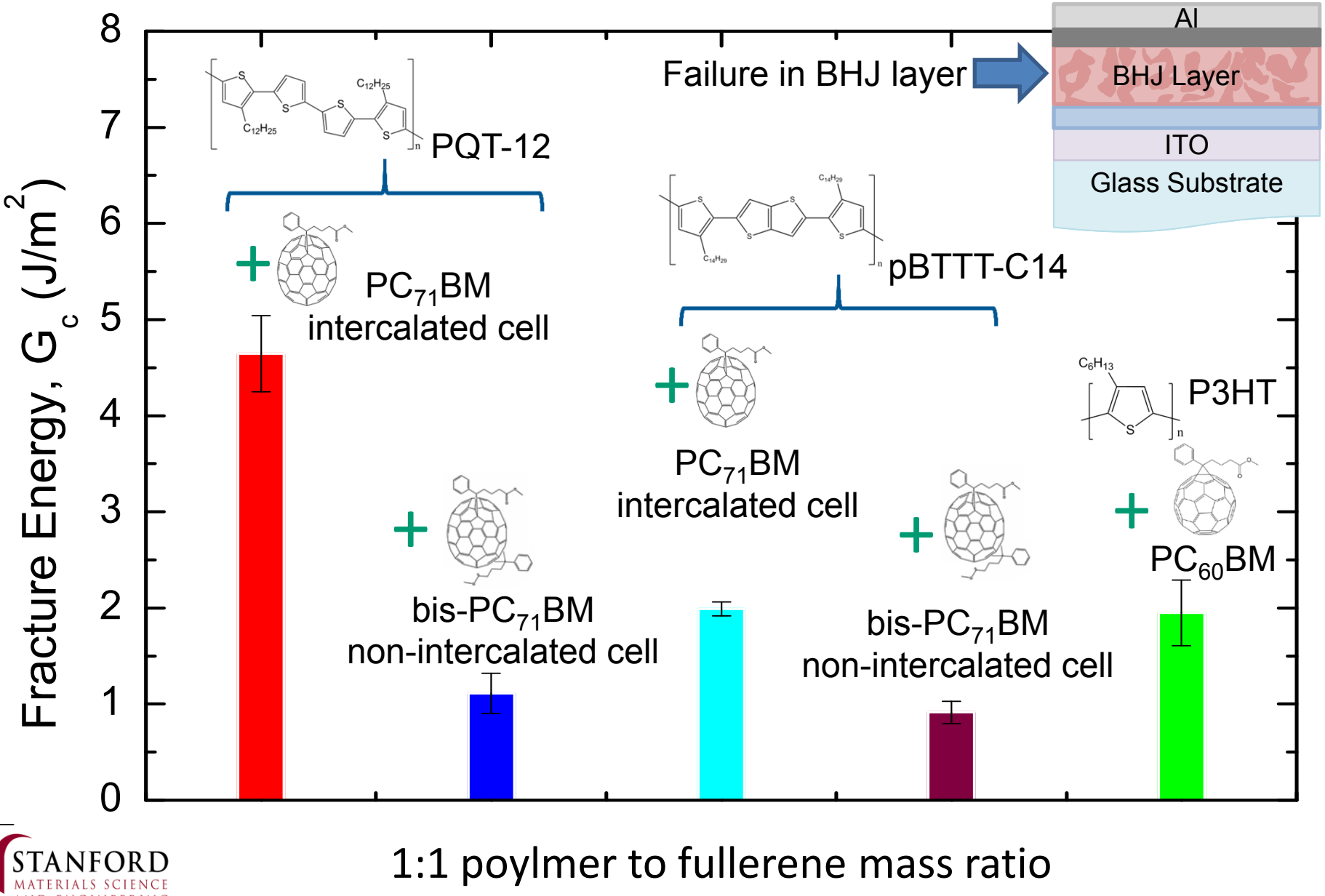
Effect of Molecular Intercalation on Cohesion



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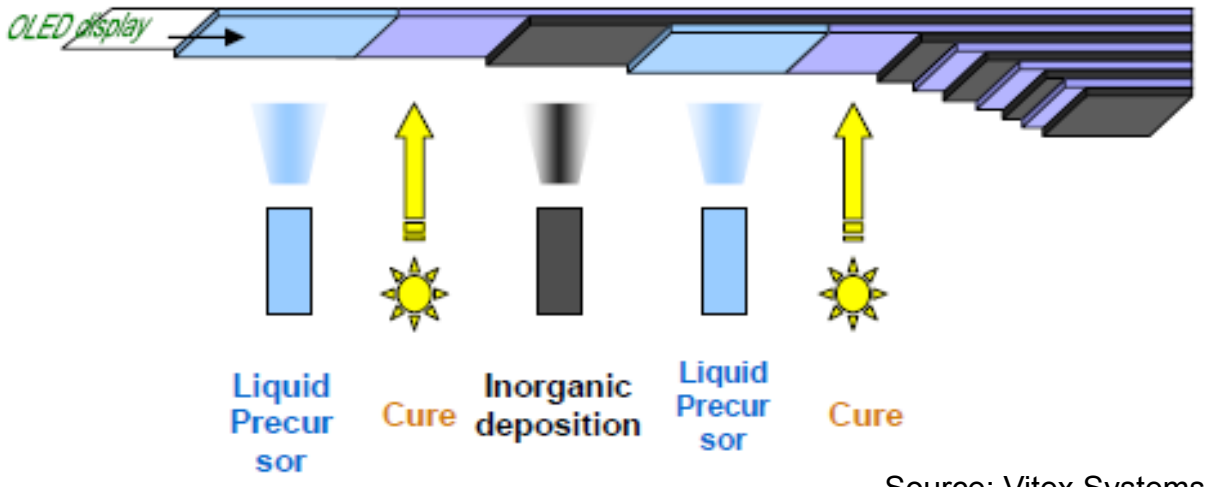
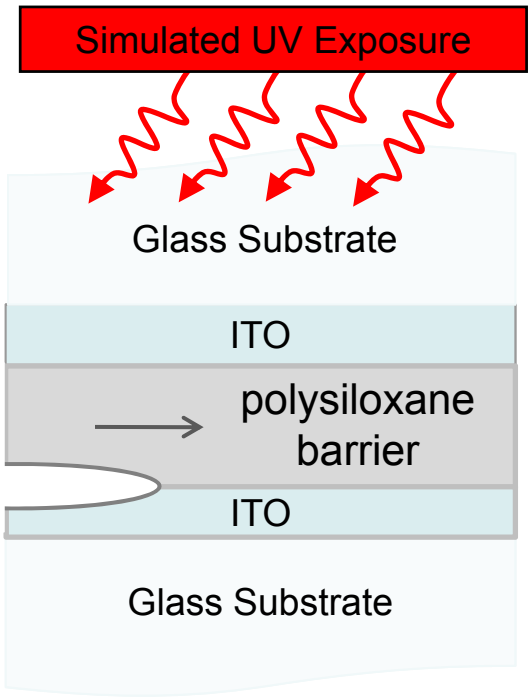
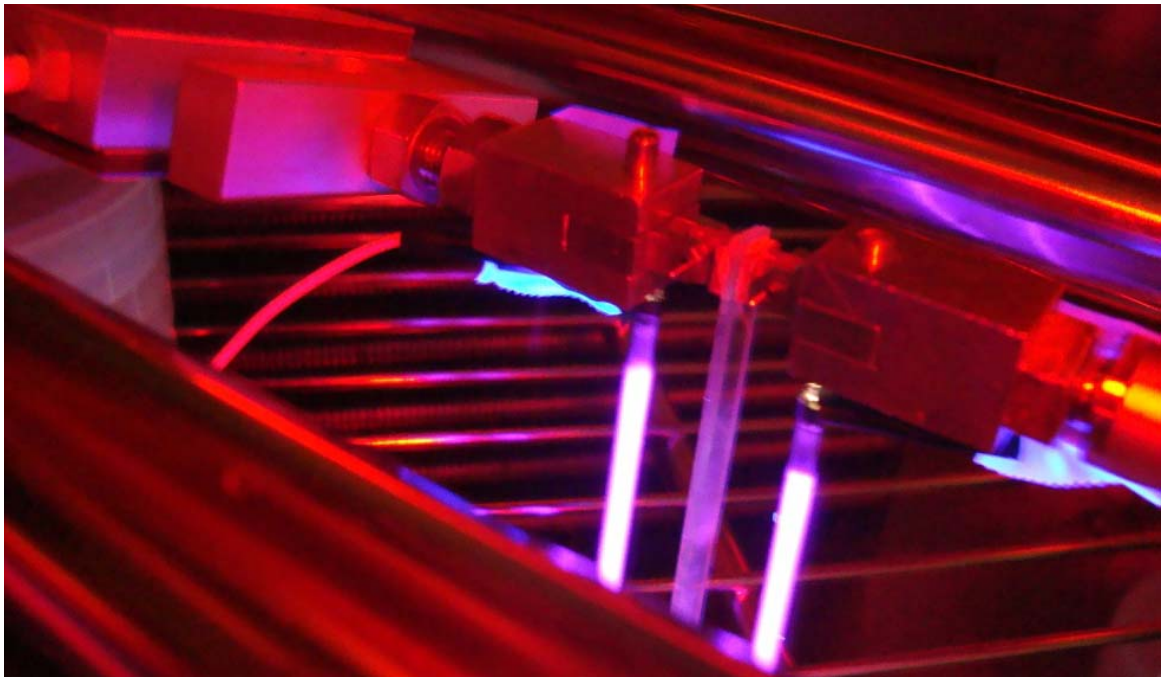
Barrier Films in Solar Modules

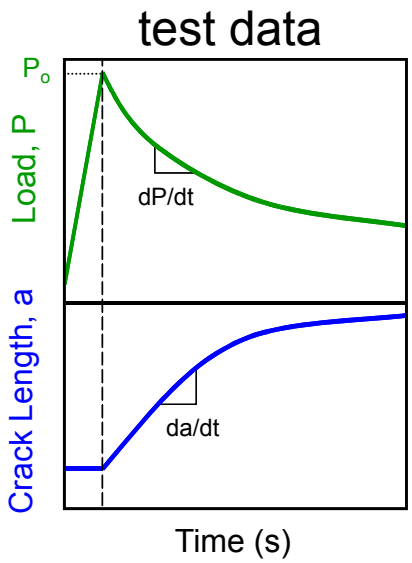


Source: Vitex Systems

Assessing UV and Environment on Debonding Kinetics







DTS Delaminator v8.2 automated load relaxation debond growth analysis

compliance analysis

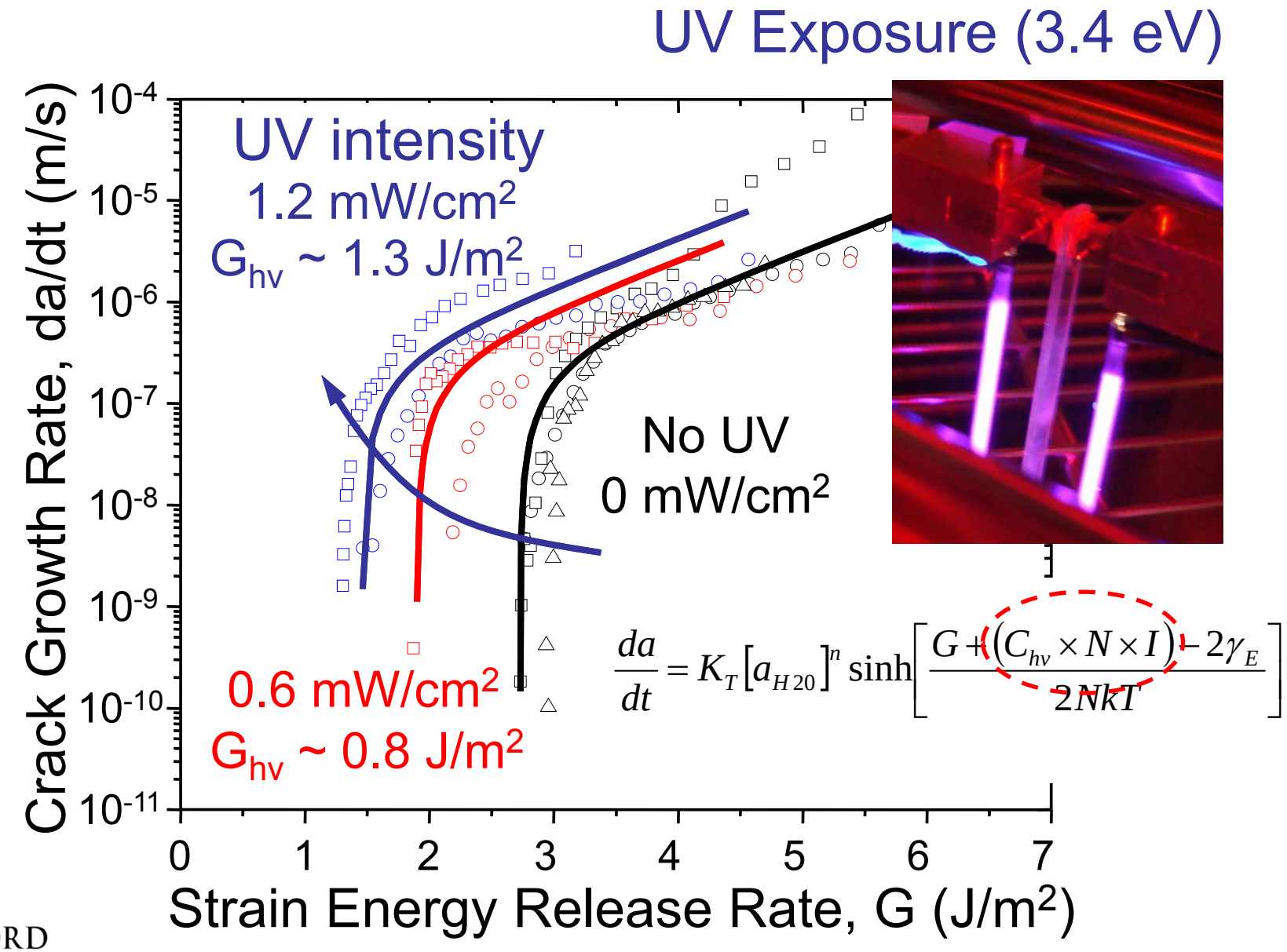
sensitivity to < 10^{-10} m/s

Debonding Kinetics

explore role of:

- UV flux
- humidity, O_2, OH, …
- temperature
- mechanical loading

UV Effects on Molecular Bond Rupture



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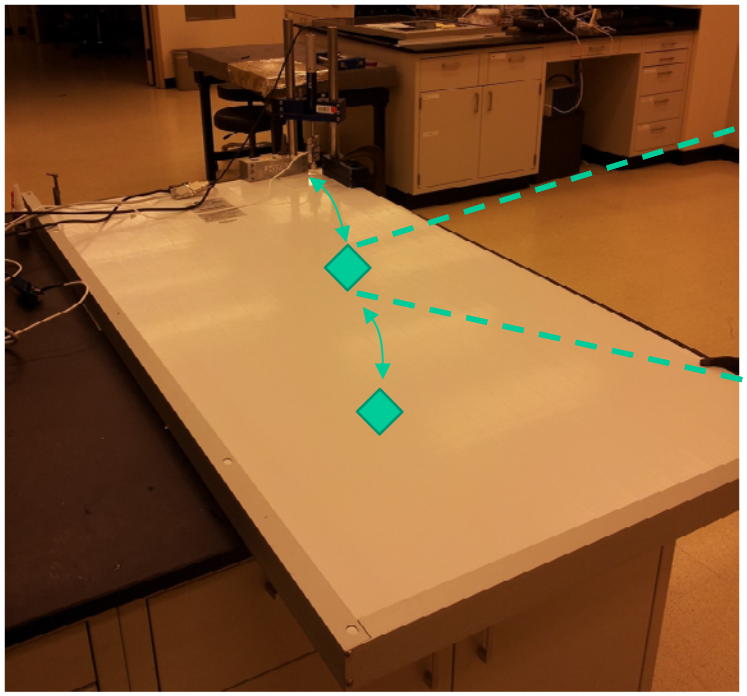
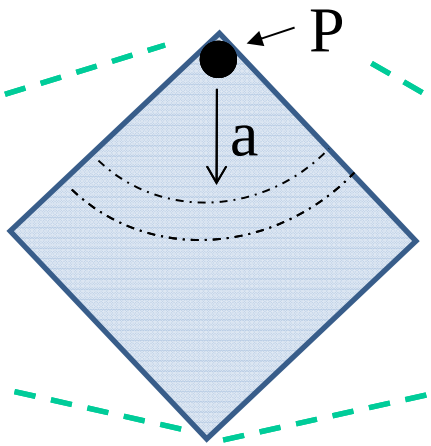
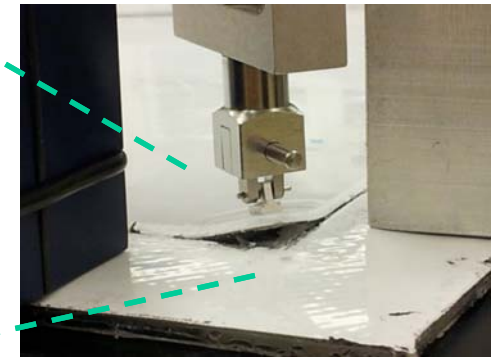
Backsheet and Encapsulant Debonding in Solar Modules

New Portable Full Panel Adhesion

Back Side of Full Panel







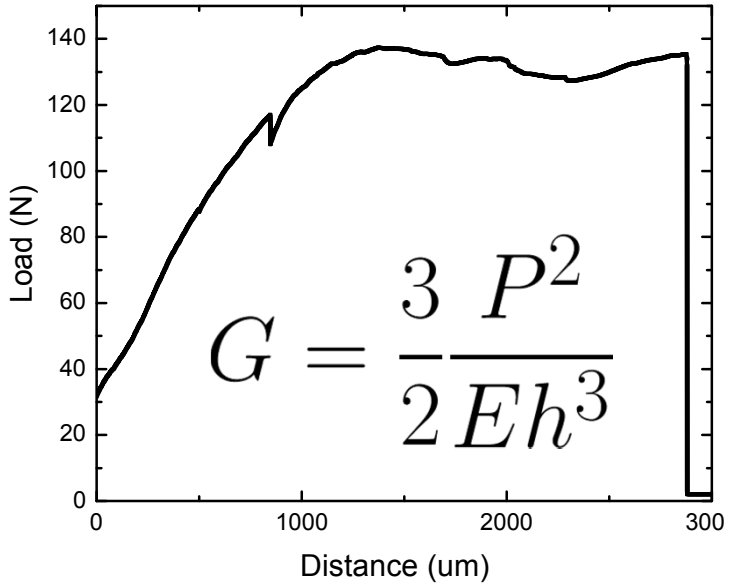
Delaminator (v8.2)
Adhesion Test System

Square Cantilever Beam Adhesion

Adhesion energy, G_c, depends on:

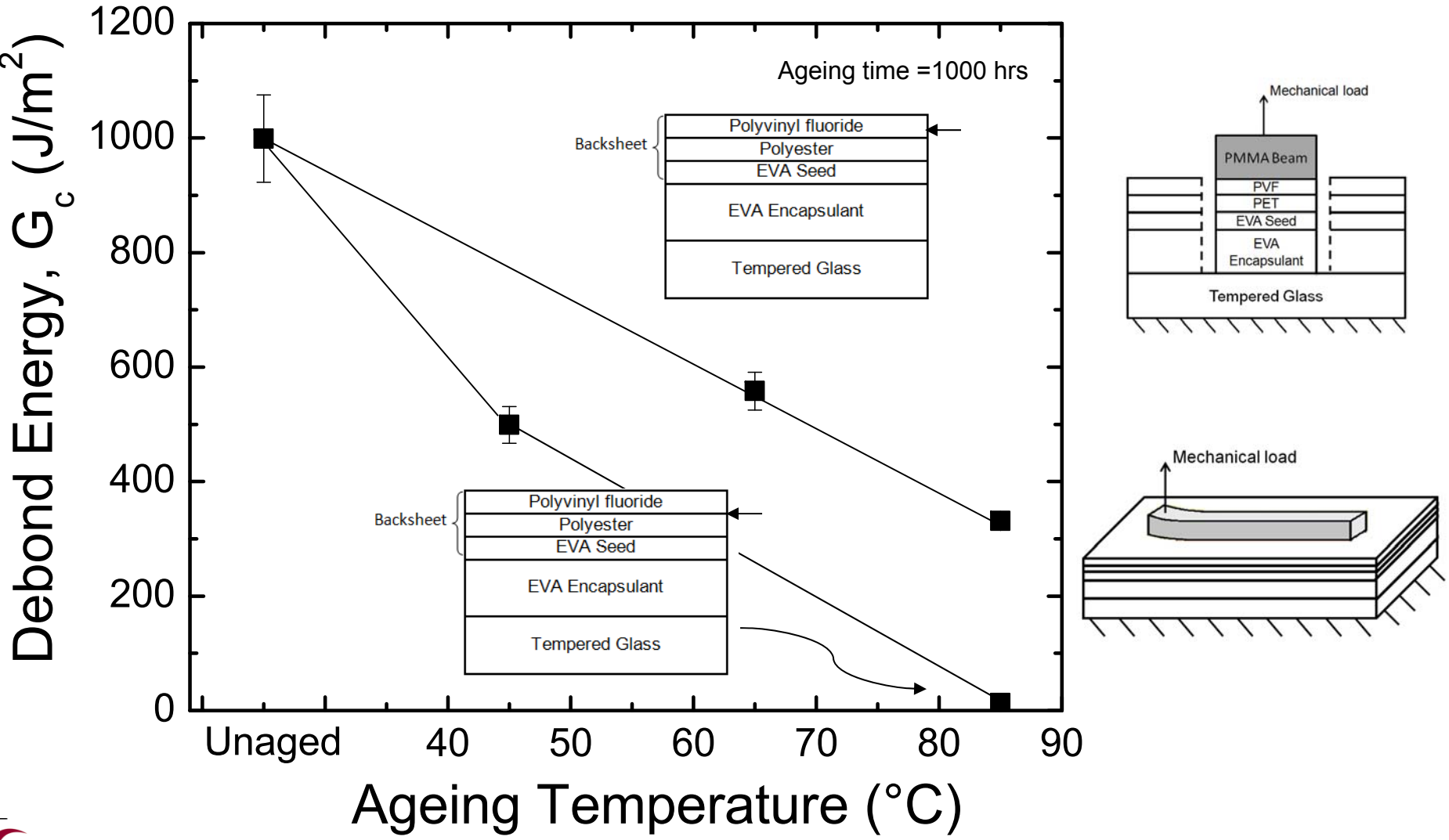
P (delamination force)
E (young modulus of the square)
h (thickness of the square)

$$G = \frac{3}{2}\frac{P^2}{Eh^3}$$



DTS system and support: dauskardt@stanford.edu

Ageing Temperature Effect on Debond Energy



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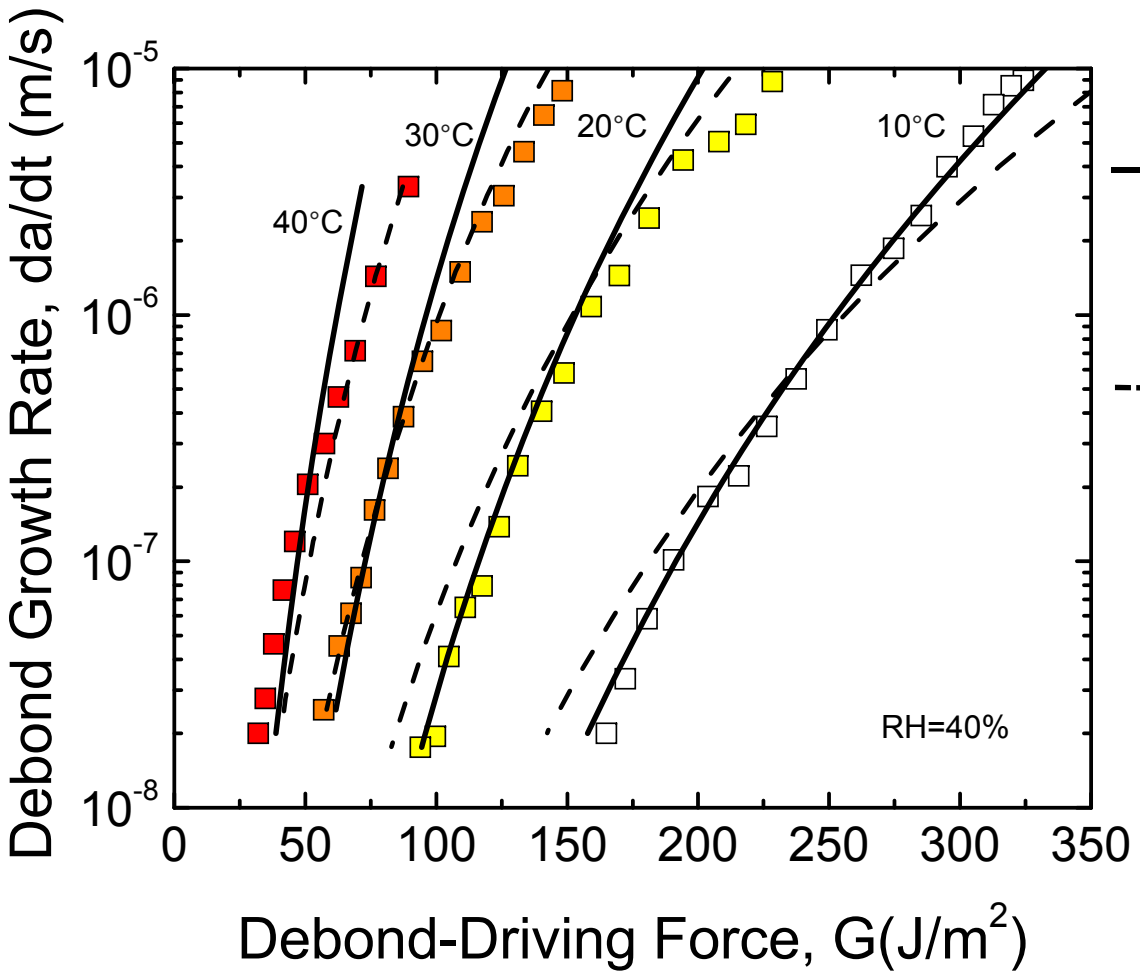
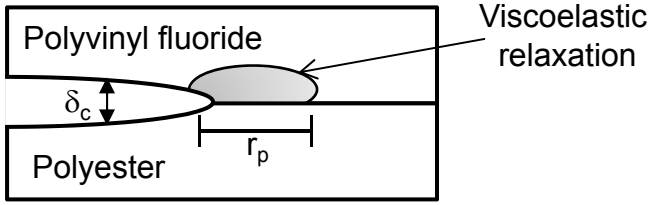
Temperature Effect on Debond Kinetics



Debond Kinetics Model

$$\frac{da}{dt} = \frac{\pi}{8}\frac{\delta_c}{\varepsilon_y(\delta_c\,\varepsilon_y)^{1/n}}\left(\frac{G}{E_0(RH)}\right)^{\frac{1}{n}} \underbrace{e^{-\frac{E_a}{R}\left(\frac{1}{T}-\frac{1}{T_r}\right)}}_{\text{Arrhenius}}$$

$$\frac{da}{dt} = \frac{\pi}{8}\frac{\delta_c}{\varepsilon_y(\delta_c\,\varepsilon_y)^{1/n}}\left(\frac{G}{E_0(RH)}\right)^{\frac{1}{n}} \underbrace{10^{\frac{C_a(T-T_g)}{C_b+(T-T_g)}}}_{\text{Williams-Landel-Ferry (1955)}}$$



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Outline

- Molecular Modeling and Design of Hybrid Glasses
  - molecular structure and mechanical properties
- High-Toughness Ceramic-Like SiC:H Films
  - toughening devices with plastic a-SiC:H layers
- Hybrid Materials in Plastic Electronics and OPV
  - cohesion and adhesion, kinetics and lifetimes
- Biological Hybrid Films and Treatments
  - biomechanics of human skin, UV exposure and treatment

Biological Hybrid Films and Treatments

http://www.npr.org/blogs/health/2012/10/02/162159367/how-sunlight-weakens-your-skin

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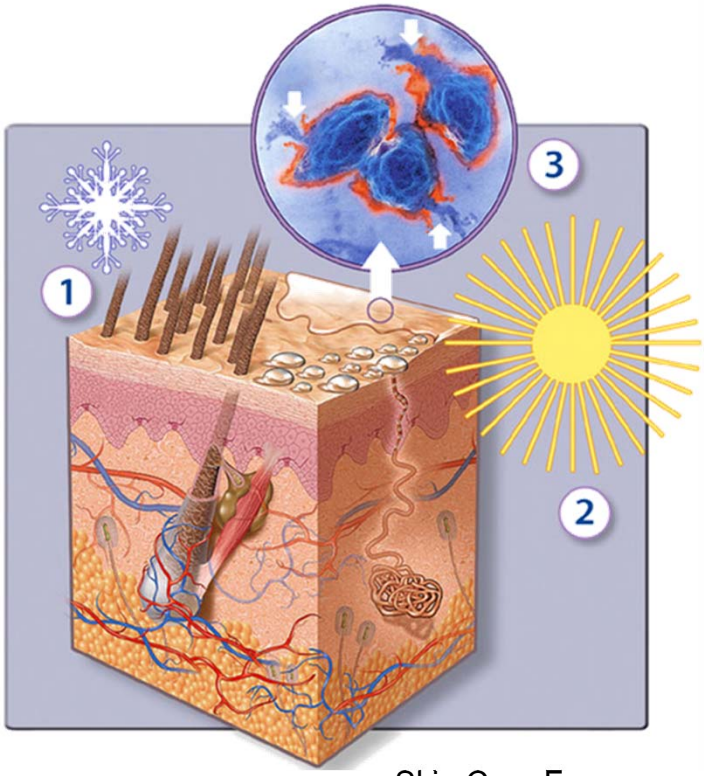
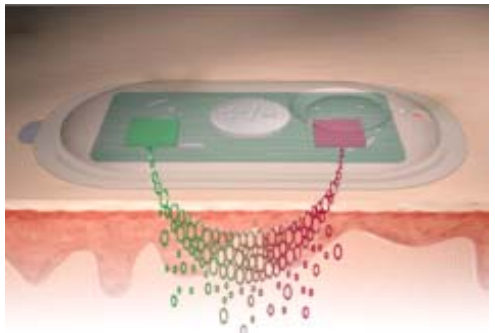
Biniek, Levi, Dauskardt, *PNAS, Oct 1, 2012*

Mechanical Function of Human Skin

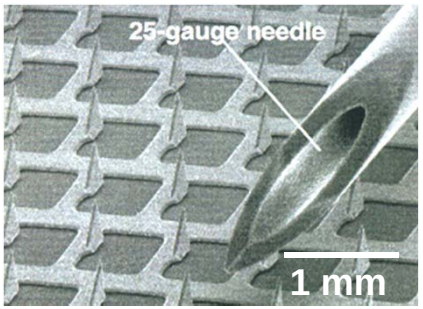


Skin Care Forum

mechanical behavior effects cosmetic aspects of skin appearance, feel, and firmness…


Alza E-Trans ®

mechanical function and solar UV exposure, wound care, biosensing, drug delivery, and scar formation…



Alza Macroflux ®

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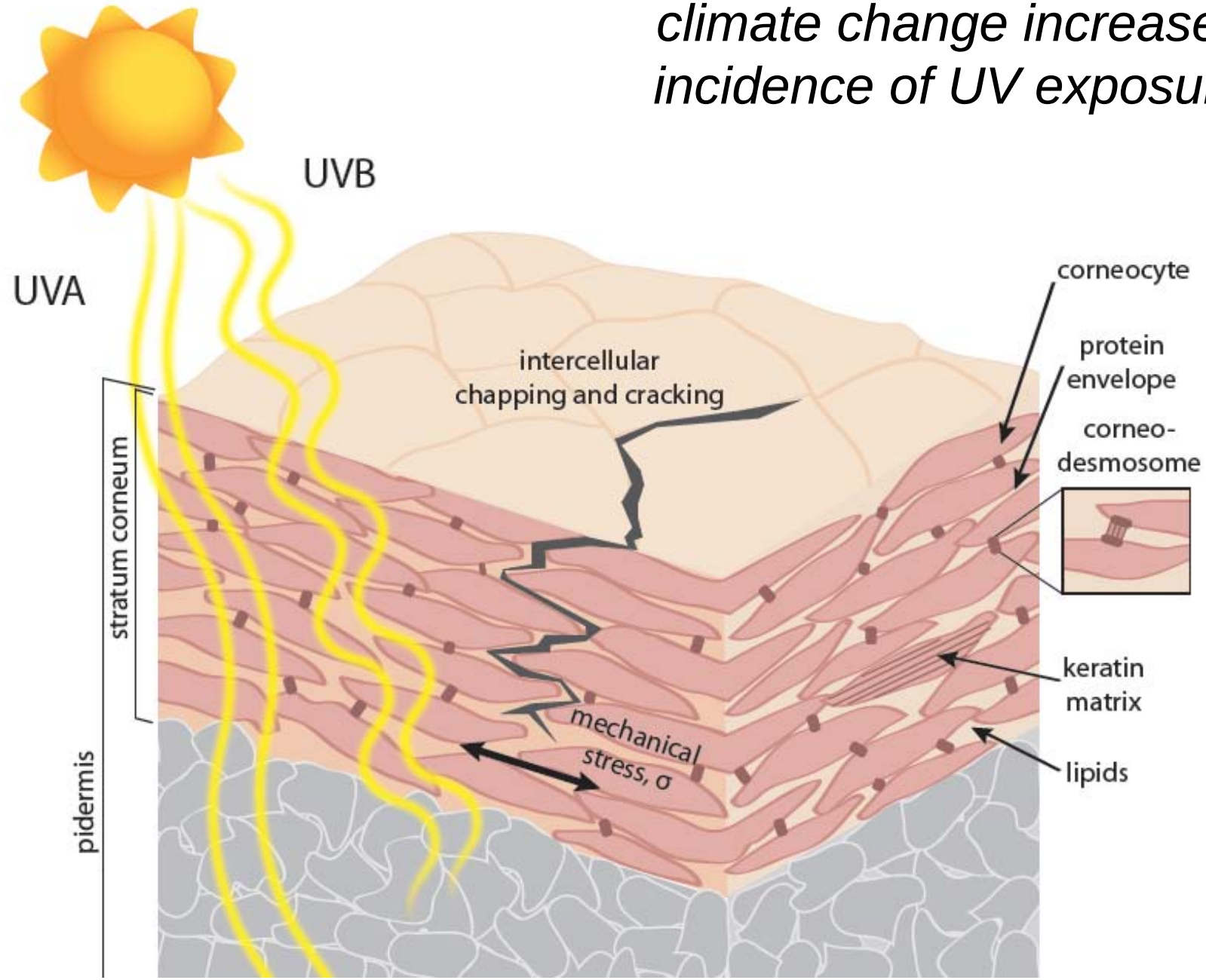
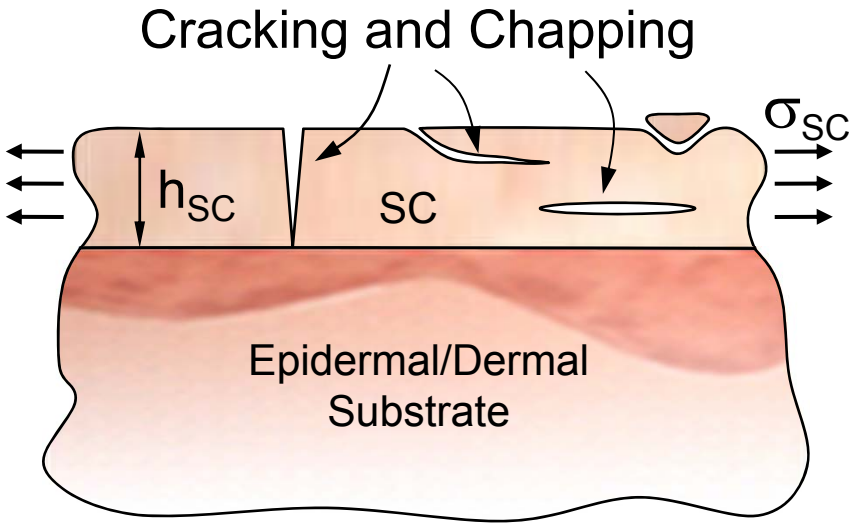
Solar UV Effects on Biomechanical Function

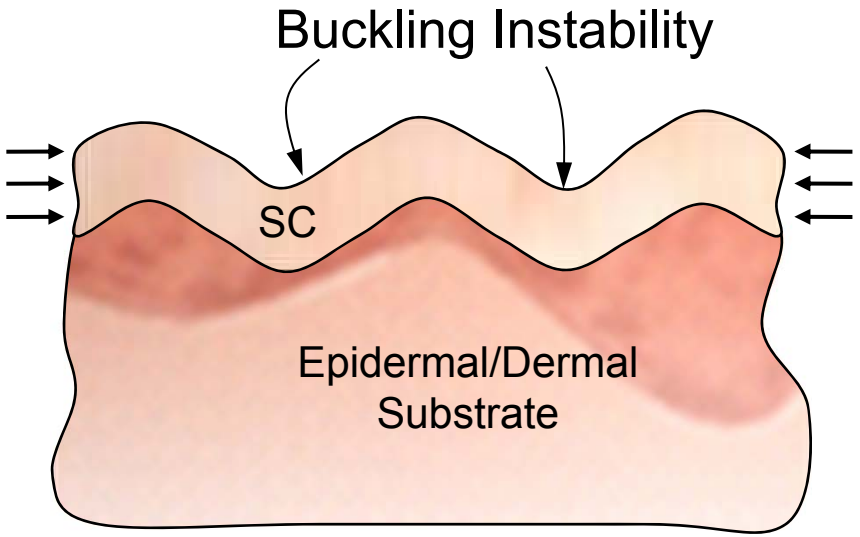
climate change increases incidence of UV exposure



Biomechanical Model for SC Damage



SC in tension



SC in compression

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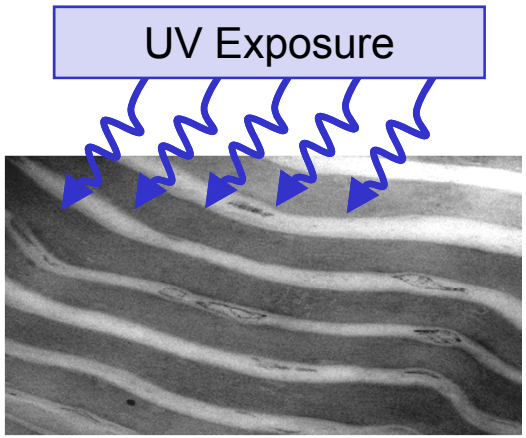
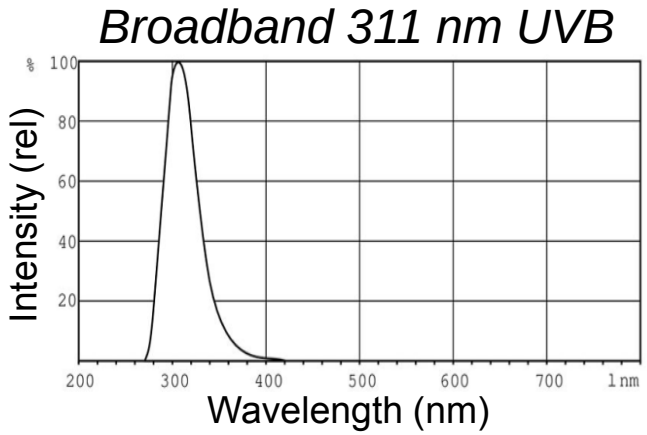
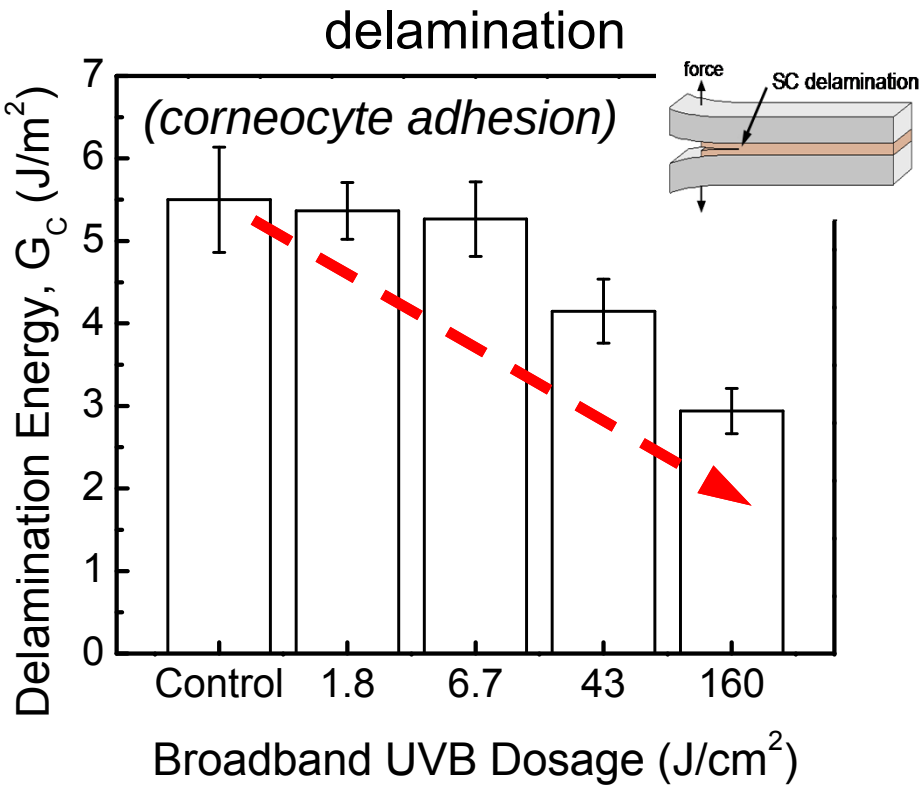
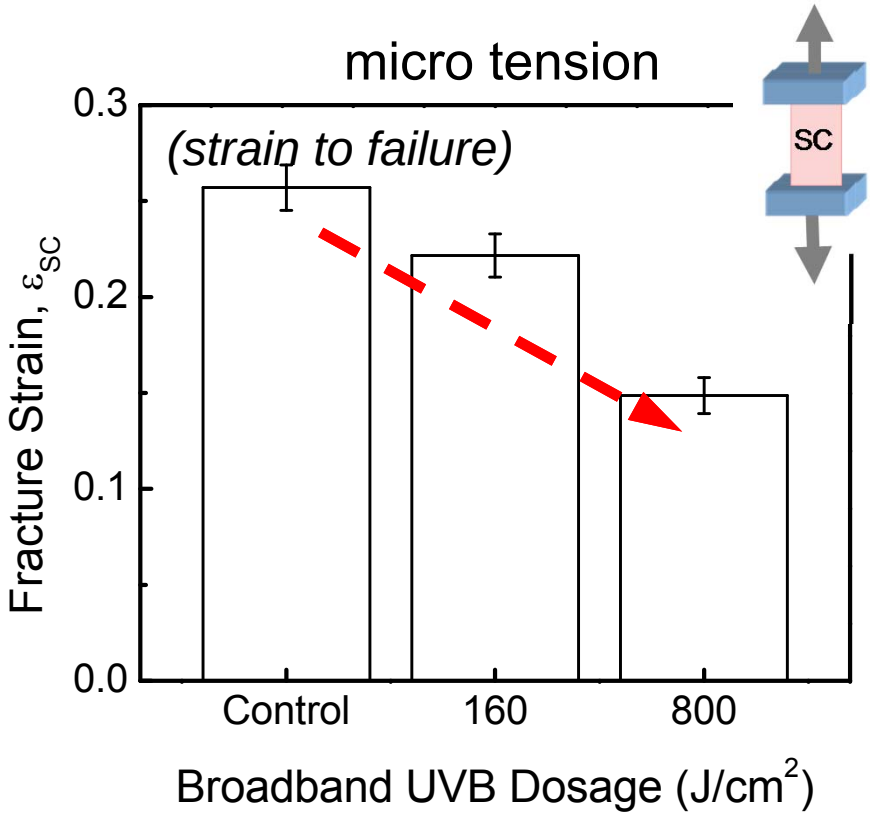
Solar UV Effects on Biomechanical Function

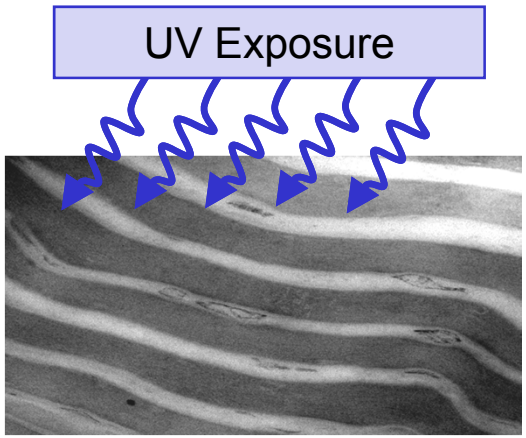






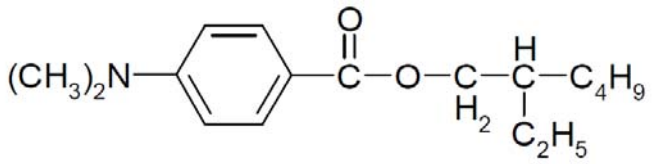


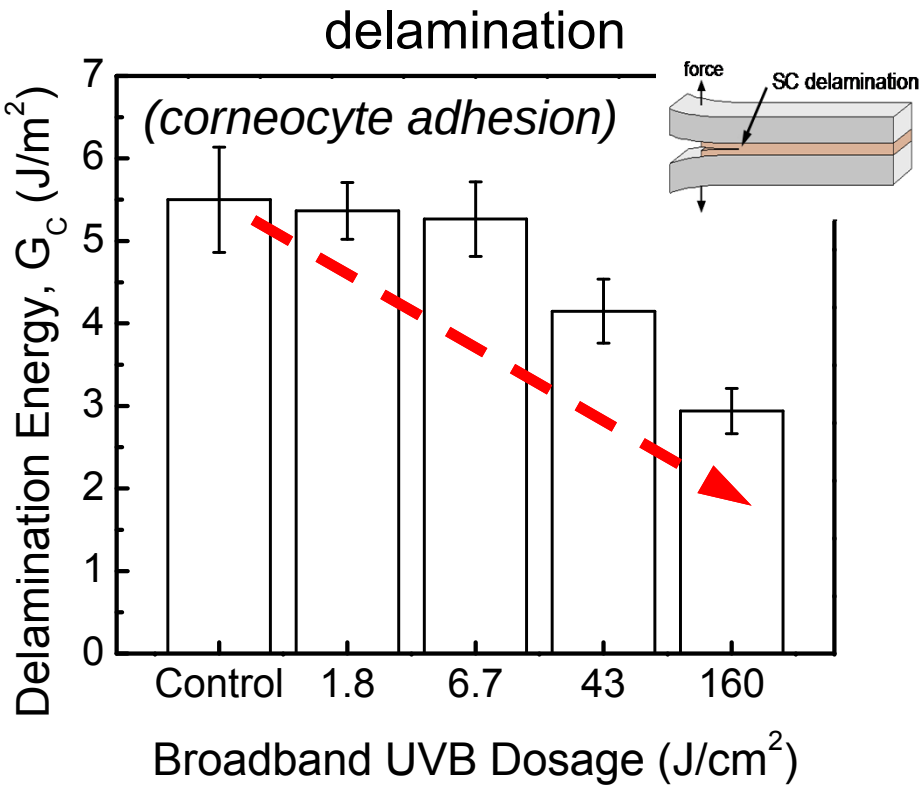
Solar UV Effects on Biomechanical Function

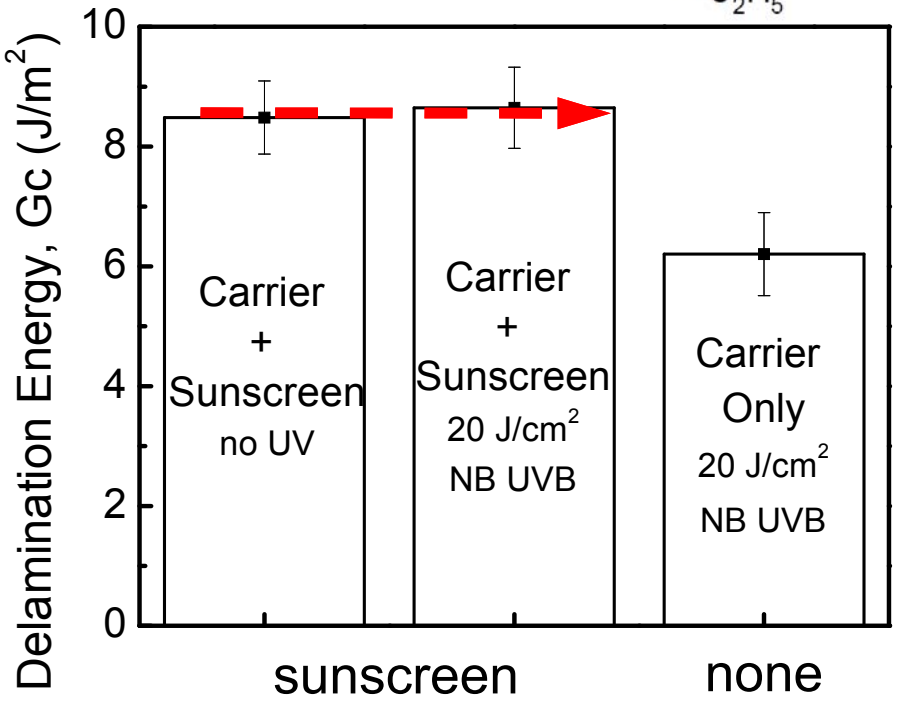


UVB Sunscreen
Carrier (Phenethyl Benzoate)
+ Sunscreen (8% Padimate O)

UVB absorber
Ethylhexyl Dimethyl PABA

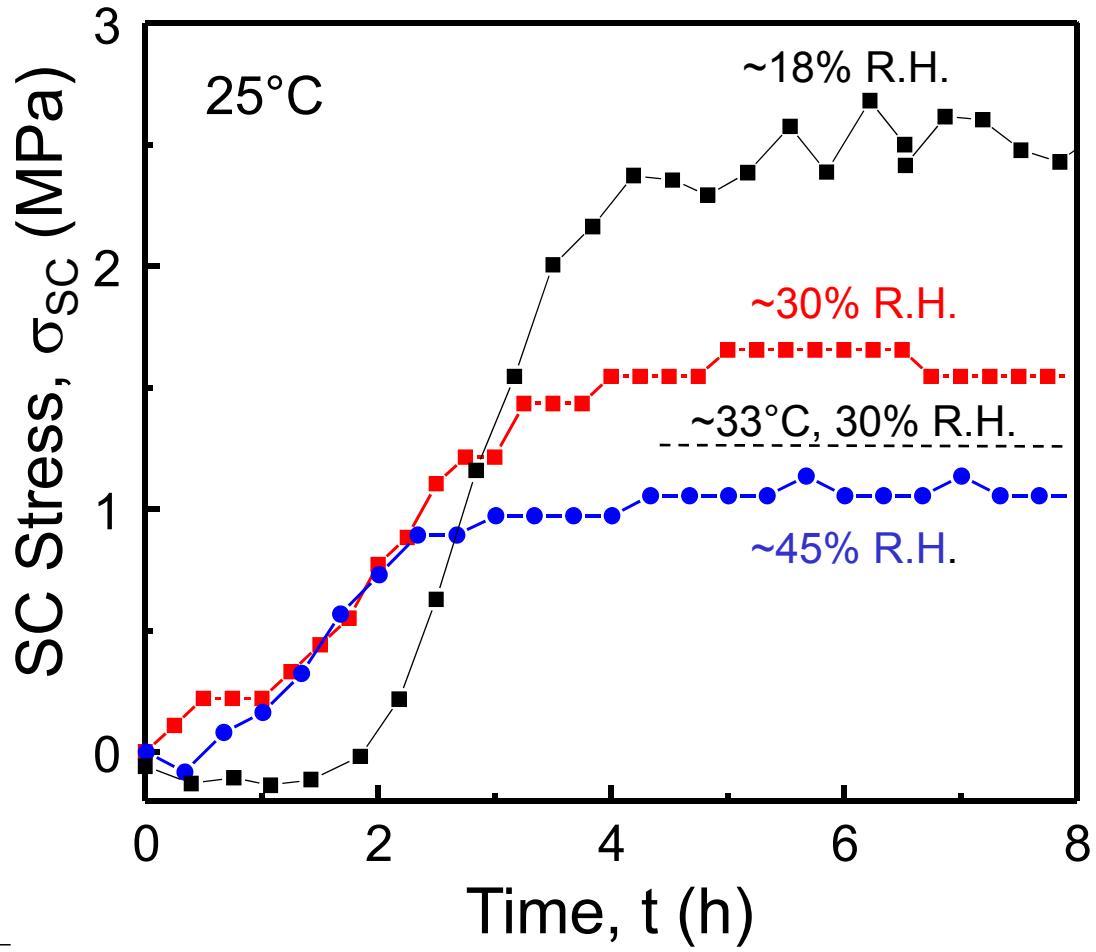




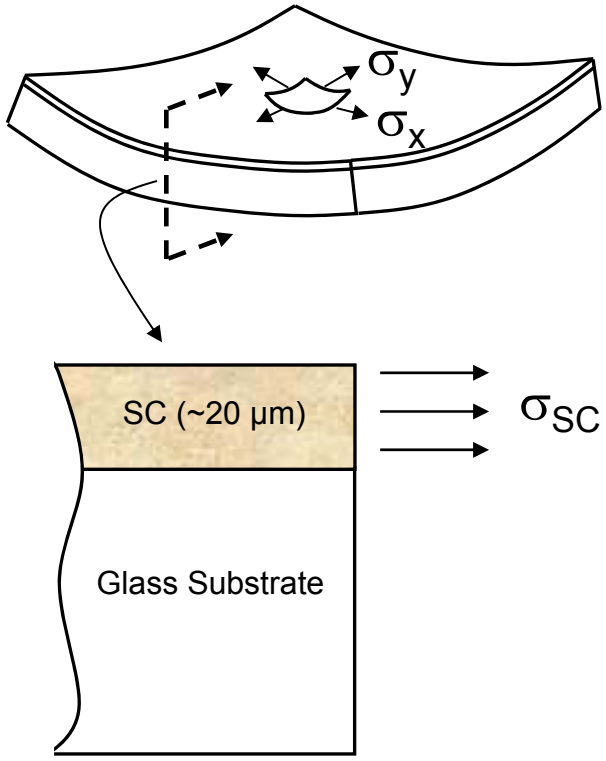


Skin Stresses and the Driving Force for Damage

- wafer curvature technique for SC stresses
- effects of treatment on stresses



In-Plane Bi-Axial Stress State

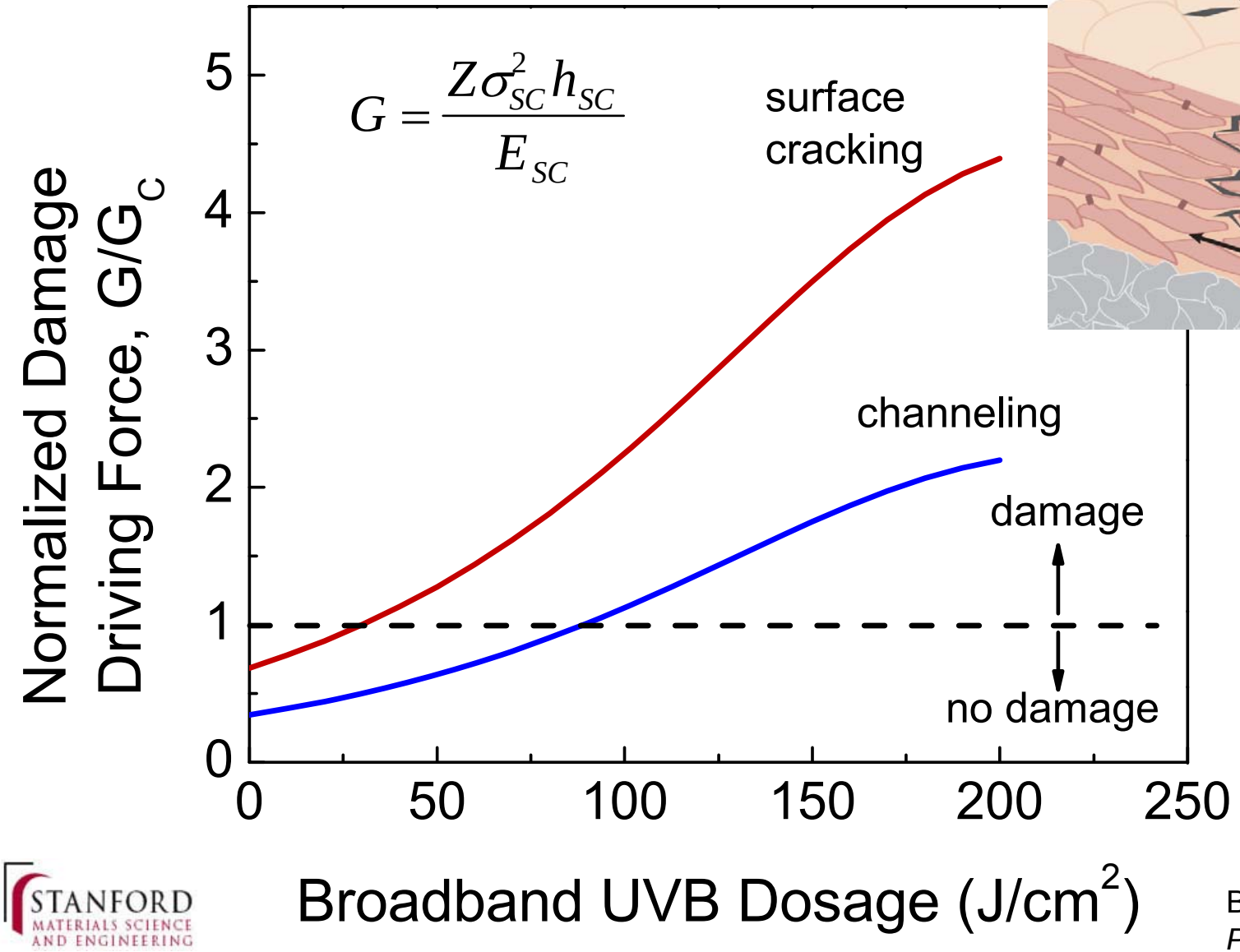


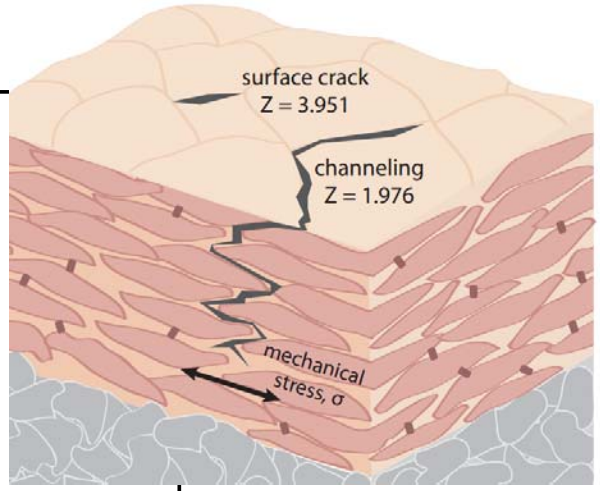
$$G = \frac{Z\,\sigma_{SC}^2\,h_{SC}}{\overline{E}_{SC}}$$

STANFORD MATERIALS SCIENCE AND ENGINEERING

Levi, Weber, Do, Dauskardt, Int. J. Cos. Sci., 2010.

Predicted UVB Effects on SC Damage





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PNAS, 2012

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