Molecular Bond Rupture Kinetics in Organic Photovoltaic Transparent Barriers

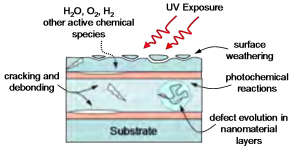
F. Novoa and R. H. Dauskardt

Objective

- The Lifetime of a Photovoltaic device is dictated by the loss of adhesion and defect evolution.
- The objective of this research is to develop quantitative methods to characterize basic thermomechanical properties (e.g. adhesion, cohesion), and photochemical and environmental degradation processes in organic solar cells.
- Kinetic models of damage evolution need to be developed as the basis for life prediction and accelerated testing (effect of operating temperature and environments, solar flux, etc.)

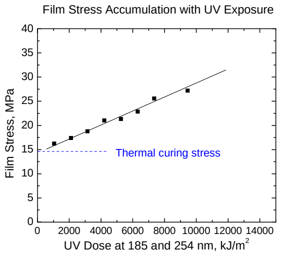
Degradation and Reliability of Photovoltaic Devices

Keele University



Locations with the highest solar irradiance are also the most severe operating environments

Exposure to moisture, chemically active environmental species, thermal cycling and UV radiation leads to device failure.



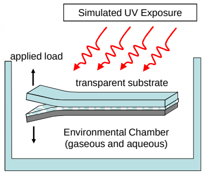
Driving force for damage:

$$G = \frac{Z\sigma_f^2 h_f}{E_f}$$

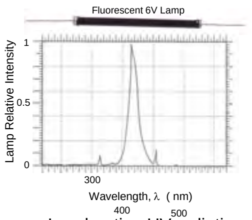
Kamer and Dauskardt - 2009

UV radiation on a polysiloxane film provides the driving force for defect propagation.

Assessing UV & Environment on Debonding Kinetics



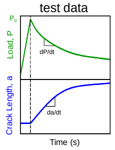
Adhesive debonding in Organic Layer



Low heating UV radiation

UV-Mechanical Delaminator

- An experimental setup was implemented to simulate effects of simultaneous environmental, mechanical and uv irradiation
- Load relaxation curves characterize the molecular bond rupture kinetics of transparent protective barriers



automated load relaxation debond growth analysis

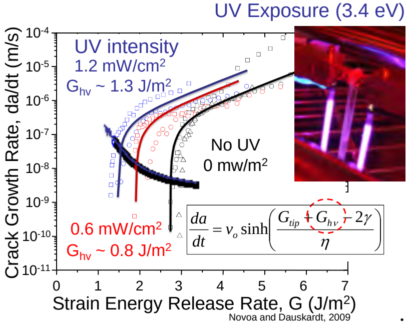
compliance analysis

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

Debonding Kinetics explore role of:

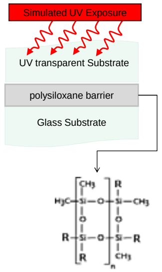
- UV flux
- humidity, O_2, OH^-, …
- temperature
- mechanical loading

UV Effects on Barrier Debonding Kinetics



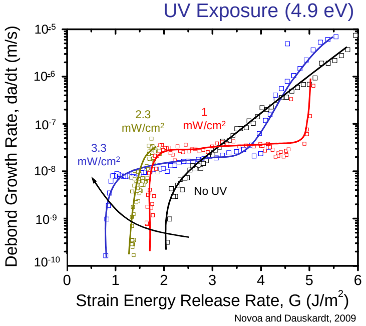
$$\frac{da}{dt} = \nu_o \sinh\left(\frac{G_{tip} + G_{h\nu} - 2\gamma}{\eta}\right)$$

3.4 eV UV light exposure accelerates debonding rates between glass and the polysiloxane barrier



Transparent Polysiloxane Barrier

- Dip coated polysiloxane coatings
- Substituted methylsiloxanes polymer with organofunctional polysiloxanes



4.9 eV UV light exposure accelerates adhesive failure while increasing bond density in the polysiloxane film

Modeling Bond Rupture Kinetics

- Interaction of moisture with strained debond tip bonds

$$nH_2O + B(\text{debond tip}) \xrightarrow{h\nu} B^*(\text{activated complex})$$

- Atomistic crack-growth models:

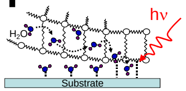
$$rate = f_o\left[\exp\left(\frac{-U_+^*}{kT}\right) - \exp\left(\frac{-U_-^*}{kT}\right)\right]$$

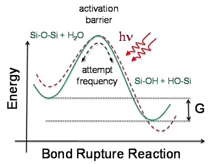
$$\frac{da}{dt} = \nu_o \sinh\left(\frac{G_{tip} + G_{h\nu} - 2\gamma}{\eta}\right)$$

$$\nu_o = \frac{2f_o}{Nw}\exp\left(\frac{-u_1}{kT}\right)$$

Bond Rupture Parameters

N - bonds per unit area, f_o - attempt frequency
u_o - work of rupture, u_1 - energy barrier
2γ - N u_o, η - 2NkT
w - crack width





UV photons cleave highly strained bonds and accelerate the rate of defect evolution

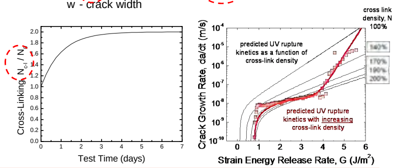
- Damage growth rate with increasing bond density:

$$\frac{da}{dt} = \nu_o \sinh\left(\frac{G_{tip} + G_{h\nu} - 2\gamma}{\eta}\right)$$

$$\nu_o = \frac{2f_o}{Nw}\exp\left(\frac{-u_1}{kT}\right)$$

Bond Rupture Parameters

N - bonds per unit area, f_o - attempt frequency
u_o - work of rupture, u_1 - energy barrier
2γ - N u_o, η - 2NkT
w - crack width



Conclusions and Future Work

- Degradation of a transparent protective barrier was shown to be caused by the simultaneous effect of moisture, chemically active environmental species and UV radiation
- UV exposure accelerates debonding rates and lowers the threshold loads for bond rupture
- More experiments on UV, humidity, environmental species and mechanical loads on bond rupture kinetics will be performed.
- Atomistic modeling to reveal bond rupture processes is under way.
- Reliability modeling and life prediction studies will be performed.

Acknowledgement

This work was supported in part by the Center for Advanced Molecular Photovoltaics (Award No KUS-C1-015-21), and by the Office of Basic Energy Sciences, Materials Sciences Division of the U.S. Department of Energy (Contract No. DE-FG02-07ER46391). FN was partially supported by a Roberto Rocca Education Program Fellowship.