Enhancing Thermal Conductivity and Mechanical Properties with Development of Porous et-OCS and Isotactic PMMA Solar Nanocomposite

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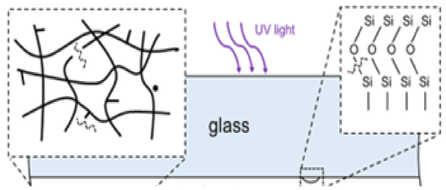
Abstract

Effective thermal management is critical for improving the performance and lifetime of solar cells. Polymers have gained attention as thermal interface materials for solar cells due to their low cost, ease of processing, and flexibility. However, their low thermal conductivity limits heat dissipation. In this computational molecular dynamics study, we develop porous oxycarbosilane with methane bridging (et-OCS) and isotactic poly(methyl methacrylate) (PMMA) with enhanced thermal conductivity due to interfacial bonding and mechanical properties for solar cell applications. Molecular dynamics simulations were conducted in order to produce nanoscale replications of an iso-PMMA - et-OCS nano composite which has been theorized to produce enhanced mechanical properties. Thermal conductivity of the PMMA has been showcased to increase by over 20% and accurate PMMA models were produced with near-identical experimental values. The improved thermal conductivity coupled with maintained mechanical performance makes these porous polymers viable thermal interface materials for efficient solar cell thermal efficiency. This computational study provides molecular-level insights into developing novel thermally conductive porous polymers coupled with organosilicates for solar cell applications.

Introduction

In this study, Molecular Dynamics is utilized to provide the ability to investigate the nano-scale of molecularly-confined nanocomposites utilizing both et-OCS and PMMA.



Schematic 1: Effect of long-term UV exposure on solar-panel deg. [1] [2]

Polymers have emerged as promising thermal interface materials for solar cells due to their low cost and flexibility

However, the intrinsically low thermal conductivity of polymers, typically 0.1-0.3 W/mK, severely limits their ability to dissipate heat from solar cells.

Fig. 1:

Isotactic Amorphous PMMA in Simulation Cell of 1.5 nm^3 after relaxation of 10 ns NPT

In addition, Organo-silicates (OSGs) have eminent potential as raw photovoltaic cell material.

However, the mechanical properties of OSGs pose concerns for mechanical longevity.

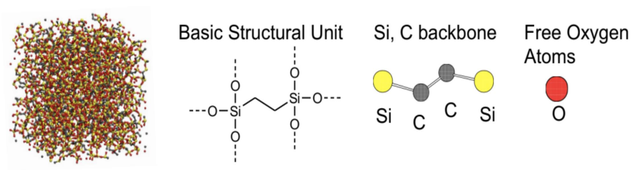


Fig. 2:
Methyl-Bridged et-OCS Organosilicate Molecular Models [2]

The prospect of an ultra-high interfacial density nanocomposite, combining the flexibility of PMMA, with the thermal conductivity of an OSG molecule (et-OCS), holds serious potential for novel solar cell materials.

Computational Methods

Et-OCS models

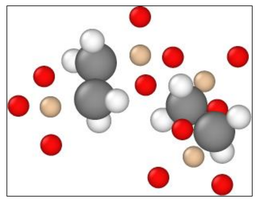


Fig. 3:
Et-OCS molecular geometry w/ Hydrogen atoms included.

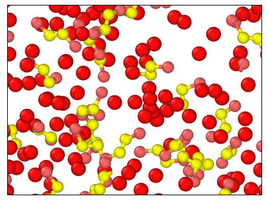


Fig. 4:
Et-OCS hybrid network with Coarse-grained Hydrogens. Stillinger Webber Potentials

PMMA models

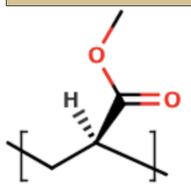


Fig. 5:
PMMA-R Isotactic Monomer

PMMA models were crafted through CHARMM-GUI
- 10 kDa MW
- 100 monomers/chain

Hybrid Force Field

$$U(r,s,\theta) = \sum_i \sum_{j>i} \phi_2(r_{ij}) + \sum_i \sum_{j\neq i} \sum_{j>k} \phi_3(r_{ij} s_{ik} \theta_{ijk})$$

$$+$$

$$V = \sum_{bonds} k_b(b-b_0)^2 + \sum_{angles} k_\theta(\theta-\theta_0)^2 + \sum_{dihedrals} k_\phi[1+\cos(n\phi-\delta)]$$
$$+ \sum_{impropers} k_\omega(\omega-\omega_0)^2 + \sum_{Urey-Bradley} k_u(u-u_0)^2$$
$$+ \sum_{nonbonded} \left(\epsilon_{ij} \left[\left(\frac{R_{min_{ij}}}{r_{ij}} \right)^{12} - 2\left(\frac{R_{min_{ij}}}{r_{ij}} \right)^{6} \right] + \frac{q_i q_j}{\epsilon_r r_{ij}} \right)$$

Stillinger-Webber Potentials & CHARMM Potentials utilized to create hybrid force field

Thermal Conductivity

$$\kappa = \frac{V}{k_B T^2} \int_0^\infty \langle J_x(0) J_x(t) \rangle \, \mathrm{d}t = \frac{V}{3k_B T^2} \int_0^\infty \langle \mathbf{J}(0) \cdot \mathbf{J}(t) \rangle \, \mathrm{d}t$$

Green-Kubo Formalism

We implemented the Green-Kubo Formalism into LAMMPS. The formula utilizes 3 Tensor Values: Stress, Potential Energy, and Kinetic Energy to find the Heat-flux. Afterwards, the heat-flux is utilized in isotropy to find Kappa.

Results

PMMA Computational Values

Temperature (K)	MD Thermal Conductivity (W x m-1 x K-1)
353.67	*0.2029*
300	*0.1899*

PMMA Experimental Values

T(K)	λ(W · m^{-1} · K^{-1})
PMMA	
314.61	0.1920
324.32	0.1940
333.89	0.1970
343.94	0.1980
353.67	0.2000

Fig. 6:
Reported experimental values from NREL

We observe promising PMMA thermal conductivity values. So much so that they are within 1% of the Experimental Values reported previously. This is a major milestone as such a close computational models will reveal critical results.

Et-OCS – PMMA Interface Results

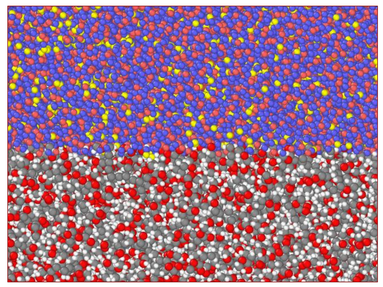


Fig. 7:
The figure to the right represents the boundary layer between the et-OCS (top) and PMMA (bottom)

Our et-OCS and PMMA thermal conductivity results yielded a **15%+** efficiency bolstering in thermal transport through the interface layer. This holds great promise for future studies

Future work

For upcoming work, we aim to utilize quartic bonds and ReaxFF models to model mechanical properties of the porous nanocomposite. With the thermal stability calculations finished, it provides opportunities for in-depth analysis of long term durability of the nanocomposite.

[1] Alan Liu, 2023 MRS

[2] Kilic, Karsu I., and Reinhold H. Dauskardt. "Computational Analysis of the Re of Nanoconfinement on the Reliability of ULK Glasses." *2022 IEEE International Interconnect Technology Conference (IITC)*. IEEE, 2022.