Laser-Induced Porous Graphene Sponge for Oil Sorption

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Motivation

- Oil spills have significant environmental, economic, and societal impacts
- Carbon-based materials show promise for oil sorption [1]
- Current technology for oil removal is not selective [1]
- A scalable, comparatively inexpensive fabrication technique for laser-induced porous graphene (LIG) was developed [2]


[5]

Objectives

- Develop a tunable porous graphene material for oil sorption
- Create atomistic and fluid flow models for oil sorption in porous graphene
- Determine a relation between pore size and oil sorption

Background

Materials for Oil Sponges

Polyurethane and Polypyrrole	99% porous Carbon Nanotube (CNT)	>90% porous Spongy Graphene (SG)
- Can absorb up to 30 grams of oil per gram of polymer [3]	- Can absorb 80 grams of oil per gram of CNT with selectivity [4]	- Can absorb up to 70 grams of oil per gram of graphene [1]
- Selective only with coating - Environmentally harmful - High volume needed	- Very expensive - Complex, resource intensive processing	

Laser-Induced Graphene

A novel method of producing porous graphene by irradiating polyimide (PI) film with a 3.6W IR laser was recently developed [2]

- Laser ablation breaks non-carbon-carbon bonds leaving porous graphene behind
- LIG porosity, pore size, and film thicknesses are controllable with process parameters
- LIG is cost effective and scalable

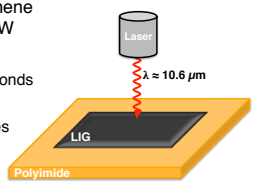


Figure 1: Schematic of LIG production on PI substrate using a 3.6W IR CO_2 laser

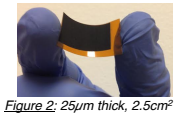


Figure 2: 25μm thick, 2.5cm² 3.6W LIG on polyimide substrate

Table 1: Pore data for 3.6W-LIG [2]

Diameter (Å)	Density (m^2g^{-1})	Proportion (%)
23.6	137.5	47
36.8	92.5	31.6
53.7	47.5	16.2
89.4	15	5.1
Total	292.5	100

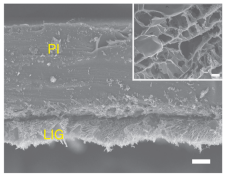


Figure 3: SEM image of LIG on the PI substrate; scale bar, 20 μm. Inset scale bar, 1 μm. [2]

Atomistic Modeling

Goal:
Understand oil-graphene interaction at the nanoscale

Energy Minimization in VASP:

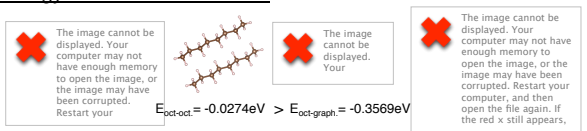


Figure 4: Interaction energies between system components. Octane-graphene is favored.

Figure 5: Lowest energy configuration of octane on graphene.

Molecular Dynamics in LAMMPS:

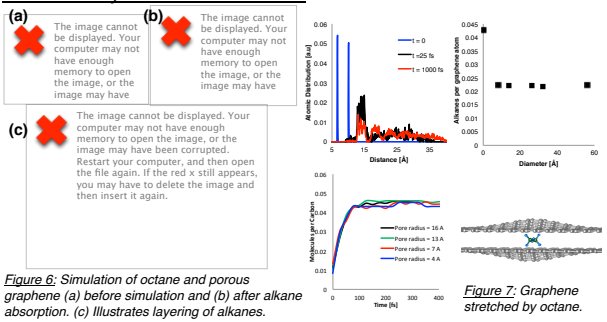


Figure 6: Simulation of octane and porous graphene (a) before simulation and (b) after alkane absorption. (c) Illustrates layering of alkanes.

Figure 7: Graphene stretched by octane.

Fluid Flow Modelling

Goal:
Implement Darcy's Law to understand bulk fluid flow through porous media.

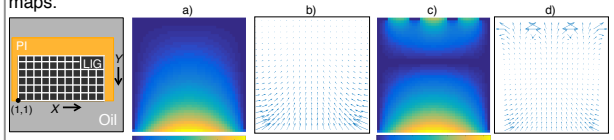
Equation:

$$\left(\frac{\partial^2\Psi}{\partial X^2}+\frac{\partial^2\Psi}{\partial Y^2}\right)=-\omega, \text{ where } U\frac{\partial\omega}{\partial X}+V\frac{\partial\omega}{\partial Y}=\frac{\varepsilon}{Re}\left(\frac{\partial^2\omega}{\partial X^2}+\frac{\partial^2\omega}{\partial Y^2}\right)-\frac{\varepsilon^2}{DaRe}\omega-\frac{F\varepsilon^2}{\sqrt{Da}}\|v\|\omega$$

Ψ = stream function; *X,Y* = coordinates; ω = vorticity; *Da* = Darcy Number; *F* = geometric function; *U,V* = interstitial velocity components; ε = porosity; *Re* = Reynolds Number; v = velocity vector (all variables are dimensionless)

Assumptions and inputs:
System initially empty (air omitted); Porosity is uniform in X and Y directions; Excluding influence of gravity; ε, *Re, Da* estimated from our system.

Results: (a,c) Steady-state stream functions, (b,d) fluid velocity vector maps.



Schematic of the System | Closed System | Closed System | Open System | Open System

Experimental

Materials
- Sample: 25μm thick, 2.4cm² 3.6W LIG on polyimide substrate
- Oil: 99% anhydrous n-octane
- Microbalance: 0.001 ± 0.01 mg

Experimental results:
- Porous graphene only absorbs nonpolar octane and not polar water
- The sorption capacity of LIG is about 8 grams of oil per gram of graphene
- Samples exhibit capillary action when partially submerged in octane
- Absorption may be surface-only due to linear dependence with time

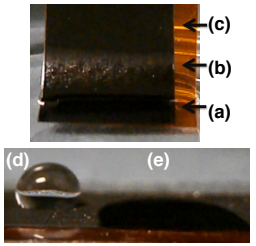


Figure 8: Capillary action of oil, with (a) oil, (b) wet graphene, and (c) dry graphene. Example of (d) hydrophobicity and (e) oil sorption of LIG.

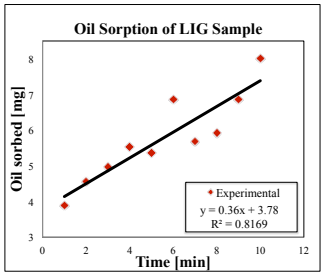


Figure 9: Graph of oil sorption over time. The trend is linear, suggesting surface absorption

Conclusions

- LIG absorbs fewer grams of oil per gram of graphene
- Oil sorption is independent of pore size
- Distinct octane layers formed over porous graphene sheets
- Sheet spacing is not sufficient for bulk oil sorption
- In its current state, LIG is not a marketable oil sponge

Future Work

- Fabricate ideal design using open backside of LIG
- Test LIG with different pore characteristics
- Implement crude oil in sorption tests
- Increase sheet spacing of LIG
- Investigate mechanical stability of LIG

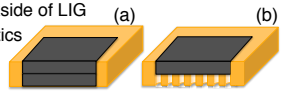


Figure 10: Schematic of idea designs: (a) entire cross-section LIG, (b) LIG on porous PI substrate

References

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