Multiscale study of the thermophysical properties of polymeric nanocomposite materials

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Master Programs: CODS Connected Objects, Devices and Systems

ESIEE Programs: ENE, SEI, SE

A. Master internship proposal

Context and motivations:

Global climate change is now unmistakably apparent and largely irreversible, primarily due to a combination of historical and ongoing human activities.¹ Recent research¹ underscores the fact that nearly all of the world's energy consumption involves processes related to the production or manipulation of heat across a broad spectrum of temperatures. Consequently, the effective management of thermal energy has emerged as a central concern in our global energy production and consumption landscape. Given the critical juncture of our societal and environmental development, there is an urgent need to introduce innovative and alternative solutions for energy management. The proposed research critically examines distinct approaches aimed at fine-tuning the thermal conductivity and enhancing the properties of polymer based solid materials, suitable for applications including, electric vehicles, portable electronics, or data centers, where efficient heat dissipation is required.

The development of novel materials using carbonaceous nanomaterials such as graphene to precisely control thermal conductivity, surpassing that of currently employed materials, is indispensable for influencing the performance and reliability of the aforementioned applications.^{2–6} One promising avenue involves the utilization or creation of nanostructured or nanocomposite materials, as they offer the potential for finely-tailored thermal conductivity. These cutting-edge, human-engineered materials are considered among the most promising materials of our generation.^{7–10} Realizing their full potential necessitates an interdisciplinary approach involving thermal engineering optimization and the establishment of design principles. Furthermore, it calls for the implementation of dual methodologies, combining multiscale models for predicting material properties with specifically tailored experimental characterization techniques and methodologies.

Objectives

This research endeavor focuses on the experimental synthesis and examination of the relationship between microstructure and thermophysical attributes in polymeric materials, a relationship that hinges on the kinetics governing their transformation. The study seeks to

characterize these materials through various techniques, such as Scanning Thermal Microscopy (SThM)^{11,12} and the 3-omega method,¹³ to quantify their thermophysical properties with different spatial resolutions. Additionally, their optical properties, particularly emissivity, will be assessed using Infrared Fourier Transform (FTIR) spectroscopy.¹⁴

The research comprises two key phases. The initial phase involves the production of these innovative metamaterials, and the methodology for preparing such nanocomposites has already been established within the laboratory of Professor Bozlar at the University of Texas. Subsequently, the focus will shift to characterizing these novel samples, with a specific emphasis on quantifying their infrared emissions and establishing radiative properties, primarily emissivity. Emissivity, a critical radiative thermal property, holds immense relevance in various energy management applications, including radiative cooling, solar cells, infrared photodetectors, and broad-spectrum optical sources. Furthermore, the thermal conductivity of these materials will be assessed using either the SThM or the 3-omega technique, whenever applicable.

The research student's initial responsibilities will entail assisting with specific tasks in the project's early stages, progressing to the production and comprehensive characterization of these newly developed material. It's important to note that the properties of polymeric nanocomposites are intricately tied to the fabrication process and the degree of mixing between nanofillers and the polymer matrix, rendering them tunable. The insights gained from this work are anticipated to enhance our understanding of the conductive and radiative properties of these materials, potentially opening doors to their utilization in various cutting-edge applications like thermal management in electronic systems, or even radiative cooling in the built environment to reduced Air Conditioning loads.

Master internship Program:

The work plan includes the following five main steps.

- 1. Understanding the project goals through bibliography research at ESYCOM lab at the beginning of the project
- 2. Learning to use the 3-omega technique and the FTIR spectroscopy and performing experiments and measurements at ESIEE Paris, while at ESYCOM lab for the first six months,
- 3. Learning to use the SThM technique and performing experiments and measurements at CETHIL, for the last 3 months of the internship.
- 4. Experimental synthesis and analysis of the microstructure of polymeric nanocomposites at the University of Texas at Arlington (Dept. of Mechanical & Aerospace Engineering) first part of the internship for 3 months at the USA,
- 5. Examining the relationship between microstructure and thermophysical properties of samples. This step comprises also bibliography research.

B. Brief scientific description of the teams involved

Groups involved:

The project brings together leading experts in the areas of the fabrication of novel materials using carbonaceous nanomaterials, the thermal characterization and the optical measurement.

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ESYCOM Laboratory works mainly in the fields of engineering of communication systems, sensors and microsystems for the city, the environment and the person.

The topics covered are more specifically:

- Micro-devices for recovering ambient mechanical, thermal or electromagnetic energy.
- Antennas and propagation in complex media, photonic components microwaves;
- Microsystems for environmental analysis and pollution control, for health and the interface with living organisms;

CETHIL, INSA Lyon – Université de Lyon; « Micro and Nanoscale Heat Transfer » team The scientific interests of the team deal with the development of metrologies and modeling to study physical mechanisms and properties of energy transport in nanostructured objects and at solid-solid interfaces. Nanoscale heat conduction, thermoelectric generation, thermophotovoltaic devices and near-field thermal radiation are the main research topics. The team has extensive skills in Scanning thermal microscopy (SThM) and thermal analysis at micro/nanoscale. The team developed four SThM instruments and the associated measurement methodologies. S. Gomès (CNRS Prof.), who will participate in the internship supervision, is expert in SThM.

BNL, University of Texas at Arlington

Bozlar Nanoscience Lab is a multidisciplinary materials science research group. The primary goal is addressing urgent societal needs by combining fundamental and applied research, especially in the area of energy and the environment. Research at BNL is concentrated in the area of nanomaterials synthesis, characterization, and applications.

References:

- 1. Iyengar, E. v. Review: An Inconvenient Truth: The Planetary Emergency of Global Warming and What We Can Do about It, by Al Gore. *Am Biol Teach* **69**, 58–58 (2007).
- 2. Zhao, B., Hu, M., Ao, X., Chen, N. & Pei, G. Radiative cooling: A review of fundamentals, materials, applications, and prospects. *Appl Energy* **236**, 489–513 (2019).
- 3. Zhang, Y. *et al.* Recent advanced thermal interfacial materials: A review of conducting mechanisms and parameters of carbon materials. *Carbon* vol. 142 445–460 Preprint at https://doi.org/10.1016/i.carbon.2018.10.077 (2019).
- 4. Zalba, B., Marín, J. M., Cabeza, L. F. & Mehling, H. Review on thermal energy storage with phase change: Materials, heat transfer analysis and applications. *Appl Therm Eng* **23**, 251–283 (2003).
- Xu, Z. Heat transport in low-dimensional materials: A review and perspective. Theoretical and Applied Mechanics Letters vol. 6 113–121 Preprint at https://doi.org/10.1016/j.taml.2016.04.002 (2016).
- 6. Bozlar, M. *et al.* Carbon nanotube microarchitectures for enhanced thermal conduction at ultralow mass fraction in polymer composites. *Advanced Materials* **22**, 1654–1658 (2010).
- 7. Lionetto, F. & Espinoza-González, C. Emerging polymer-based nanocomposites. *Nanomaterials and Nanotechnology* **12**, 1–5 (2022).
- 8. Huang, C., Qian, X. & Yang, R. Thermal conductivity of polymers and polymer nanocomposites. *Materials Science and Engineering R: Reports* **132**, 1–22 (2018).
- 9. Ahlatcioglu Ozerol, E., Bozlar, M., Bulent Ustundag, C. & Dikici, B. Latex-Based Carbon Nanotube Composites BT Handbook of Carbon Nanotubes. in *Handbook of Carbon Nanotubes* (eds. Abraham, J., Thomas, S. & Kalarikkal, N.) 1–24 (Springer International Publishing, 2020). doi:10.1007/978-3-319-70614-6 9-1.

- 10. Luo, Y. *et al.* Active building envelope systems toward renewable and sustainable energy. *Renewable and Sustainable Energy Reviews* **104**, 470–491 (2019).
- 11. Gomès, S., Assy, A. & Chapuis, P. O. Scanning thermal microscopy: A review. *Physica Status Solidi (A)* **212**, 477–494 (2015).
- 12. Sun, W. *et al.* Investigation of the thermal conductivity enhancement mechanism of polymer composites with carbon-based fillers by scanning thermal microscopy. *AIP Adv* **12**, 105303 (2022).
- 13. Boussatour, G. *et al.* Measurement of the thermal conductivity of flexible biosourced polymers using the 3-omega method. *Polym Test* **70**, 503–510 (2018).
- 14. Del Campo, L., Prez-Sáez, R. B., Esquisabel, X., Fernández, I. & Tello, M. J. New experimental device for infrared spectral directional emissivity measurements in a controlled environment. *Review of Scientific Instruments* 77, (2006).