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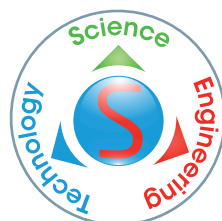
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# Design, Synthesis and Photophysical Properties of Substituted Trichlorotriphenylmethyl-based Radicals

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## Abstract:

Organic light-emitting diodes (OLEDs) have gained widespread attention in both scientific research and commercial applications due to their low cost, flexibility, environmental friendliness, and ease of processing. For traditional closed-shell molecular systems, according to quantum spin statistics, electrons and holes recombine in the luminescent layer at a ratio of 1:3 to form singlet and triplet excitons. OLEDs can only utilize up to 25% of singlet excitons for luminescence, while the triplet excitons, which account for up to 75%, are usually non-luminescent due to spin prohibition, resulting in a large amount of wasted excitons. There are well-known strategies for utilizing triplet excitons such as triplet–triplet annihilation (TTA), hybridized local and charge-transfer (HLCT) and thermally activated delayed fluorescence (TADF), but these systems all have downsides like device life and stable working efficiency. Unlike focusing on closed-shell systems, a promising direction is to use open-shell radical systems as emission layers. Radical molecules have an unpaired electron, and both their ground state and excited state are doublet states, which can avoid the problem of triplet exciton transition forbiddance and theoretically achieve 100% internal quantum efficiency without intersystem crossing. Triphenylmethyl-based radicals are one of the few types of radicals with relatively high stability. Introducing electron donors as substituents on trichlorotriphenylmethyl (TTM) radicals to design donor–acceptor (D-A) type molecules is a widely adopted strategy to improve radical stability and quantum efficiency [1].

**Keywords:** TTM; radical; OLED; emission

**Acknowledgment:** This project has received funding from the Research Council of Lithuania (LMTLT), agreement No S-MIP-24-1.

## References:

1. Li, P.; Bai, F. (2024) Thorough Examination of the Variables Affecting the Quantum Efficiency of Radiative Decay of Trichlorotriphenylmethyl Radicals. *J. Phys. Chem. A.*, 128, 4279–4287

# Photoluminescence Lifetime Dynamics in Carbon Quantum Dots: Role of Precursors, Surface States and Purification

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## Abstract:

Carbon quantum dots (CQDs) have attracted significant attention due to their size-dependent photoluminescence and complex emission mechanisms, which are strongly influenced by surface chemistry and defect states. In this work, CQDs synthesized via a bottom-up hydrothermal approach from urea–citric acid and piperazine–phthalic acid precursor systems were investigated with particular emphasis on their photoluminescence lifetime dynamics.

Time-resolved photoluminescence measurements are currently being employed to analyze radiative and non-radiative recombination processes and to evaluate the contribution of different emissive states. The effect of post-synthesis dialysis was systematically examined, as this purification step plays a key role in modifying surface-related species and low-molecular-weight fluorophores, which can strongly affect emission decay behavior. Lifetime analysis was correlated with steady-state photoluminescence, UV–Vis absorption, ATR-FTIR spectroscopy, and transmission electron microscopy in order to establish structure–property relationships.

Preliminary results indicate that both precursor chemistry and purification strategies significantly influence emission lifetimes, suggesting different recombination pathways associated with core and surface states. These findings provide fundamental insights into CQD emission mechanisms and represent an essential step toward the development of stable solid-state luminescent systems for advanced photonic technologies.

**Keywords:** carbon quantum dots, photoluminescence lifetime, time-resolved spectroscopy, surface states, recombination dynamics, solid-state luminescence, nanophotonics.

# Compositional Engineering and Advanced Investigations of Sol–Gel Derived CZTS Kesterite Thin Films

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## Abstract:

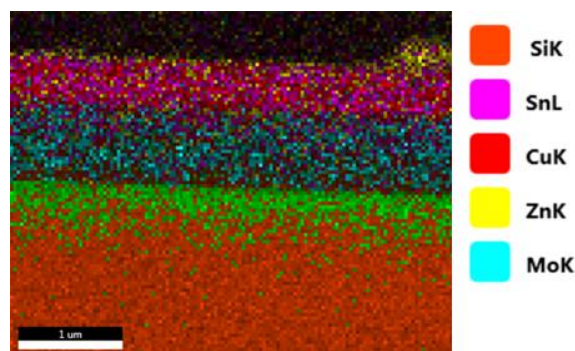
Cu<sub>2</sub>ZnSnS<sub>4</sub> (CZTS) kesterite thin films were synthesized using a solution-based sol–gel spin-coating technique, aiming to evaluate the influence of compositional gradients on their structural, morphological, and optical properties. The cationic composition was systematically tuned by varying the Cu/(Zn+Sn) ratio from stoichiometric conditions to Cu-poor regimes (0.9 and 0.8), while maintaining a constant Cu/Sn ratio of 1.6 and adjusting the Zn/Sn ratio between 1.1 and 1.3. Thin films were deposited on Mo-coated soda-lime glass substrates and subjected to controlled thermal treatments to promote crystallization.

Grazing-incidence X-ray diffraction analysis confirmed the formation of a single-phase cubic CZTS structure across all compositions, with no detectable secondary phases. Rietveld refinement revealed that decreasing the Cu content enhances crystallinity while reducing the average crystallite size, indicating modified nucleation and growth mechanisms. Morphological investigation by scanning electron microscopy showed compact, uniform, and crack-free films consisting of nanoscale grains (3–14 nm), with good adhesion to the substrate. Cross-sectional analysis highlighted a significant increase in film thickness, from approximately 359 nm to 542 nm, as the Cu/(Zn+Sn) ratio decreased.

Optical characterization demonstrated strong absorption in the visible spectral range, along with additional absorption features in the ultraviolet region (~260 nm) and extended absorption beyond 800 nm, indicating sensitivity to near-infrared radiation. These findings confirm the potential applicability of CZTS films in photovoltaic devices as well as in infrared-related technologies. Overall, the study

highlights the critical role of compositional control in tuning the microstructural and optical properties of CZTS thin films, providing a viable pathway for optimizing kesterite-based absorber layers for sustainable solar energy conversion.

**Keywords:** Cu<sub>2</sub>ZnSnS<sub>4</sub> (CZTS), kesterite thin films, compositional gradient, sol–gel spin coating, optical properties.



**Figure 1:** Elemental mapping of Cu<sub>2</sub>ZnSnS<sub>4</sub> (CZTS) kesterite thin films

## References:

1. Boerasu, I.; Vasile, B.S. (2022), Current Status of the Open-Circuit Voltage of Kesterite CZTS Absorber Layers for Photovoltaic Applications - Part I, a Review. *Materials*, 15(23), 8427.

# Preparation of Polymer Films with Hierarchically Ordered Surface Structure and their Thermo-Responsive and Adhesive Properties

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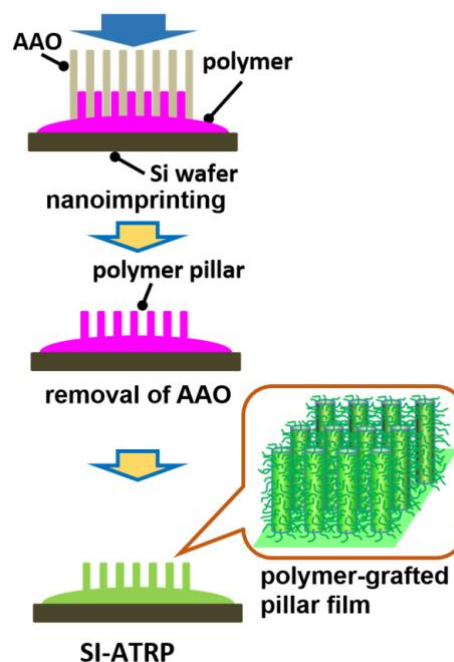
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## Abstract:

Recently, various types of biomimicry materials have attracted much attention due to their remarkable surface functions. Polymer films with submicron-sized complex surface structures have been produced by top-down approaches (e.g. nanoimprinting) or bottom-up approaches (e.g. surface-initiated graft polymerization). Here, we have developed a new methodology for the preparation of polymer films with hierarchically ordered surface structure by combining nanoimprinting and surface-initiated ATRP (SI-ATRP), and investigated their thermo-responsive and adhesive surface properties. To obtain the films, nanoimprinting was firstly achieved by employing a polymer having both cross-linkable moieties and ATRP initiating sites and an anodically-oxidized porous alumina (AAO) as a template. After removal of AAO and subsequent cross-linking by photoirradiation, the films having vertically oriented polymer pillars on their surfaces were formed. Finally, the films were subjected to SI-ATRP of several monomers to give the target polymer-grafted pillar films (Fig. 1). The precursor copolymer was obtained by free radical copolymerization of coumarin-substituted methacrylate (MCMA) and  $\alpha$ -haloester-containing methacrylate (HEMA-Br). Subsequent nanoimprinting was performed by employing AAO (Whatman® Anodisc13). After removal of AAO, the films having polymer pillars on their surfaces were obtained. The films were then photoirradiated to fix the pillar structure by intermolecular cross-linking. Finally, graft polymerization of N-isopropylacrylamide (NIPAM) or [2-(methacryloxy)ethyl]trimethylammonium chloride (MTAC) or 3-sulfopropyl methacrylate potassium salt (SPMK) on the pillar surfaces was performed through SI-ATRP under appropriate conditions. Successful preparations of the target films with polyNIPAM- or polyMTAC- or polySPMK-grafted polymer pillars on their surfaces were confirmed. To investigate the surface properties of the grafted-pillar films, the polyNIPAM- or polyMTAC- or polySPMK-grafted flat films were also prepared from the thin film of the precursor poly(MCMA-co-HEMA-Br) without pillar structure. As a result, the

polyNIPAM-grafted pillar film exhibited more significant hydrophilic-hydrophobic changes depending on temperature compared to the grafted flat film. As for the adhesion property between the cationic polyMTAC- and anionic polySPMK-grafted pillar films, greater adhesive strength was observed compared the pair of the grafted flat films. These surface properties of the grafted-pillar films are probably due to the synergistic effect of the inherent temperature responsiveness or Coulomb attraction and the characteristic pillar structure.

**Keywords:** polymer films, hierarchically ordered surface structure, surface-initiated ATRP, thermo-responsive property, adhesive property.



**Figure 1:** Preparation of the polymer-grafted pillar film.

## Reference:

1. Minoda, M., Shimizu, D., Nohara, T., Motoyanagi, J. (2025) Surface-Functionalized Polymer Films Having Hierarchically Ordered Structure by a Combination of Nanoimprinting and Controlled Graft Polymerization, *Surfaces*, 8(3), 48-59.

# Surface micro/nanostructuring of of Inconel 617 superalloy by Femtosecond Laser micromachining technology

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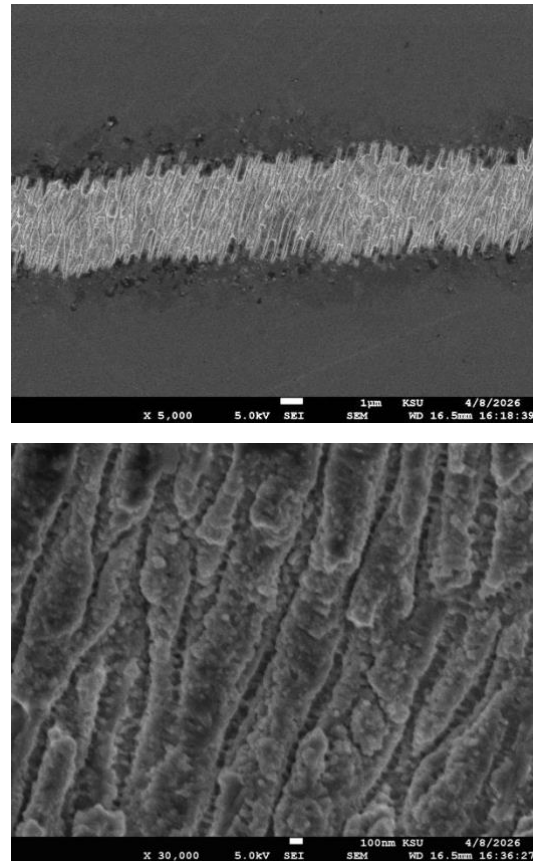
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<sup>2</sup> King Abdullah Institute for nanotechnology, King Saud University, Riyadh, Saudi Arabia

## Abstract:

Nickel superalloys, particularly Inconel 617, are widely used in high-temperature and corrosive environments due to their high stability and enhanced mechanical strength. However, improving their surface properties could be crucial to the advancement of their physical properties. As conventional modification methods are limited, advanced micro/nano surface engineering approaches are required. Femtosecond laser micromachining is a promising technology for high-precision surface modification due to its ultrashort pulse duration, high peak intensity, and ability to generate highly controlled micro and nanoscale features. This research work is aimed to fabricate micro and nanostructures patterns on the surface of the INCONEL 617 superalloy. Femtosecond laser with parameters of a wavelength of 1028 nm, repetition rate of 100 kHz, 220 fs pulse duration, scan speed of 1 mm/s, and different average laser powers in the range of 8-500 mW was used in this study. The low laser powers produced periodic surface nanostructures while the high pulse energies produced V-shape microgrooves. Finally, this technique enables the fabrication of complex surface morphologies, including laser-induced periodic surface structures (LIPSS), micro grooves, micro pores, and multiscale hierarchical textures that can significantly influence material properties such as wettability (making the surface hydrophobic), corrosion resistance, and optical reflectance/absorbance.

**Keywords:** Inconel 617 super alloy, surface structuring, femtosecond laser micromachining, corrosion resistance, optical properties.



**Figure 1:** Two magnifications SEM images of Surface nanostructuring INCONEL 617 super using a femtosecond laser with an average laser power of 8 mW and scan speed of 1 mm/s.

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# Phase purification for enhanced room-temperature ductility in complex bulk thermoelectric materials

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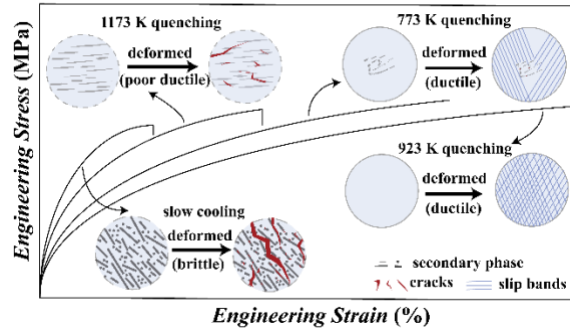
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<sup>2</sup> Center of Materials Science and Optoelectronics Engineering, University of Chinese Academy of Sciences, Beijing 100049, China

## Abstract:

Flexible thermoelectric (FTE) technology offers promise for self-powering flexible electronics based on the materials with both high thermoelectric (TE) performance and exceptional flexibility. Recently, ductile inorganic semiconductors such as  $\text{AgCu}(\text{Se},\text{S},\text{Te})$  exhibit remarkable room-temperature ductility and high TE performance, but their compositional and structural complexity often lead to detrimental phase complexity and sometime secondary phases, which greatly hinder the fundamental study and real applications. In this work, we systematically investigate the critical role of phase purity in enhancing both ductility and TE properties in  $\text{AgCu}(\text{Se},\text{S},\text{Te})$  materials. By precisely controlling the quenching temperature during synthesis process, the secondary phases with different microstructure (from the nanoscale to the micrometer scale) can be controllably created inside the matrix of  $\text{AgCuSe}_{0.22}\text{S}_{0.08}\text{Te}_{0.7}$ . Notably, quenching at 923 K produces a monophasic microstructure that exhibits exceptional room-temperature ductility (over 75% compressive strain, over 20% bending strain, and 15% tensile strain) while retaining excellent TE performance ( $zT = 0.3@300\text{ K}$ ,  $0.45@340\text{ K}$ ). Our results establish that targeted synthesis enabling phase purification is an effective strategy to concurrently optimize mechanical properties and TE performance in ductile inorganic semiconductors, providing a crucial roadmap for developing high-performance FTEs.

**Keywords:** synthesis process; phase purification  
Ductility; inorganic semiconductor; thermoelectric



**Figure 1:** Microstructure dependence on quenching temperature of  $\text{AgCuSe}_{0.22}\text{S}_{0.08}\text{Te}_{0.7}$ , resulting in varying mechanical properties.

## References:

1. Shen K L, Yang Q Y, Qiu P F, Zhou Z Y, Yang S Q, Wei T R, Shi X. Ductile p-type  $\text{AgCu}(\text{Se}, \text{S}, \text{Te})$  thermoelectric materials[J]. *Advanced Materials*, 2024, 36, 2407424.
2. Shen K L, Zhou Z Y, Zhou J L, Zhang Y, Huang Y L, Wu H J, Qiu P F, Shi X. Phase purification for enhanced room-temperature ductility in complex bulk thermoelectric materials[J]. *Acta Materialia*, 2026, 305, 121858.

# Crystal structure and silver diffusion pathway of thermoelectric $\text{Ag}_8\text{SnSe}_6$

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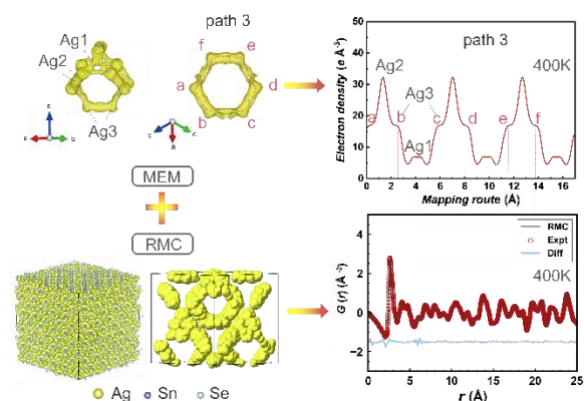
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<sup>2</sup> Center of Materials Science and Optoelectronics Engineering, University of Chinese Academy of Sciences, Beijing 100049, China

## Abstract:

Argyrodite compounds have garnered significant attention for their exceptional thermoelectric properties, with  $\text{Ag}_8\text{SnSe}_6$  standing out as a prominent high-performance material due to ultralow thermal conductivity, particularly at elevated temperatures.  $\text{Ag}_8\text{SnSe}_6$  undergoes an ordered-disordered phase transition, which leads to the formation of a three-dimensional percolation network that facilitates Ag ion transport in the disordered high-temperature phase. Despite significant progress in the thermoelectric performance of  $\text{Ag}_8\text{SnSe}_6$ , systematic experimental studies on their crystal structures, particularly the local structures along with their quantitative contribution to thermal conductivity and Ag ion migration pathways, remain limited. This work provides a comprehensive investigation into the site-specific contributions of Ag atoms to low-temperature thermal conductivity, as well as the temperature evolution during phase transitions and Ag ion diffusion at elevated temperatures. We first combine site-resolved structural, bonding and lattice-dynamics analyses with anharmonic phonon transport calculations to reveal that Ag1, Ag2 and Ag5 collectively dominate the low-frequency non-harmonic phonon vibrations, which are responsible for the ultralow  $\kappa_L$  in  $\text{Ag}_8\text{SnSe}_6$ . Then we utilize synchrotron X-ray total scattering to systematically study the crystal structure and local atomic environment, especially across the phase transition. Additionally, we combine high-quality synchrotron single-crystal diffraction with the maximum entropy method (MEM) to provide a detailed analysis of the Ag ion migration pathways for the high-temperature disordered phase. Our findings clarify the atomic-scale mechanisms underlying the ultralow  $\kappa_L$  and the specific Ag diffusion channels connecting different Ag ions in  $\text{Ag}_8\text{SnSe}_6$ , offering valuable structural insights that serve as a benchmark for understanding the thermoelectric properties.

**Keywords:** thermoelectric, characterization, argyrodite, local structure, Ag diffusion pathway.



**Figure 1:** Figure decipher and visualize the 3D percolation network of  $\text{Ag}^+$  ions via maximum entropy method, and decouple local-global dynamics structural evolution through PDFgui and reverse Monte Carlo modeling, providing critical insights into the atomic-scale origins of the ultralow thermal conductivity.

## References:

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2. Zhou, J L., Chen, X Y., Song, L R., Shen, K L., Zhang, J W., Shi, X. (2026), Protein helical structure enhancement in fluorinated-phosphonate nanoporous silica glasses characterized by circular dichroism spectroscopy Role of crystallographically distinct Ag sites in ultralow thermal conductivity of thermoelectric  $\text{Ag}_8\text{SnSe}_6$ , To be submitted.

# Mechanical Enhancement of Polyimide via Flexographic Printing of Carbon Nanostructure-Based Inks

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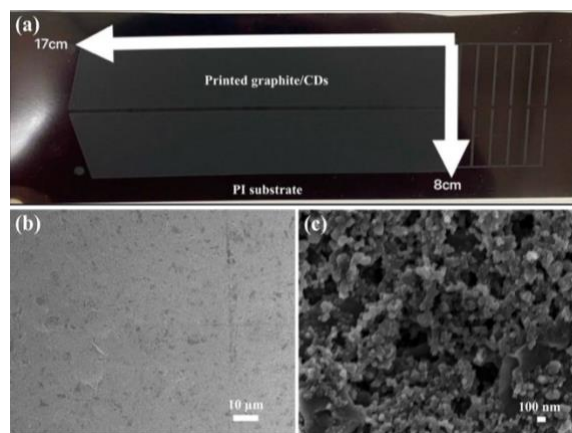
<sup>2</sup>Center of Excellence for Research in Engineering Materials (CEREM), Deanship of Scientific Research (DSR), King Saud University, Riyadh 11421, Saudi Arabia

## Abstract:

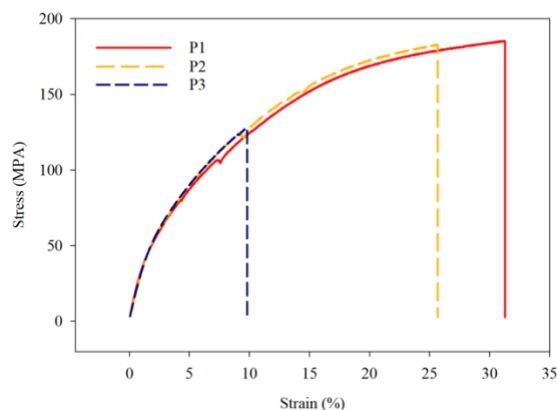
The mechanical durability of polymer substrates is a critical factor in ensuring the long-term functionality of flexible and wearable electronic devices. However, many conventional deposition and coating approaches can adversely affect substrate integrity. In this work, we investigate the potential of flexographic printing [1] as a dual-purpose technique for both patterning and mechanical enhancement of polyimide (PI) substrates using graphite/carbon dot-based conductive inks. Three sample sets were considered: printed PI (P1), PI exposed only to flexographic roller pressure (P2), and untreated PI (P3). Morphological characterization revealed consistent and uniform ink deposition, with an average thickness of approximately  $13 \pm 1.9 \mu\text{m}$ . The printed films exhibited stable electrical performance, with a measured resistance of  $475 \Omega$ , confirming the formation of continuous conductive pathways. Adhesion evaluation according to ISO 2409 indicated strong interfacial bonding (classification 1). Mechanical testing demonstrated notable improvements in the printed samples (P1), including a Young's modulus of 32.3 MPa, tensile strength of 185 MPa, and elongation at break of 31.29%. These results correspond to a 44% increase in strength and a more than threefold enhancement in ductility relative to unmodified PI. Interestingly, samples subjected solely to roller pressure (P2) also showed measurable mechanical gains, highlighting the influence of flexographic compression on substrate behavior. Nanoindentation results further supported these findings, showing increased surface hardness and improved resistance to deformation.

Overall, the results indicate that flexographic printing can serve not only as a scalable patterning method but also as an effective route for reinforcing polymer substrates, making it a promising approach for the fabrication of mechanically robust flexible electronic systems.

**Keywords:** Graphite, carbon dots, flexography printing, polyimide, mechanical properties



**Figure 1.** (a) Photograph of flexographically printed graphite/carbon dots on PI substrate. (b) SEM image showing uniform coverage of the graphite/carbon dot. (c) High-magnification SEM image showing interconnected carbon dots integrated with graphite sheets.



**Figure 2:** Stress–strain behavior of samples P1, P2, and P3 obtained from tensile testing.

## References:

1. Assaifan, A.K., et al., *Scaling-up medical technologies using flexographic printing*. *Talanta*, 2020. **219**: p. 121236.

# Biomechanical behaviour of atraumatic tool with an insert made of metamaterials

M Basiaga<sup>1\*</sup>, J Szewczenko<sup>1</sup>, W Kajzer<sup>1</sup>, K Wilk<sup>1</sup>, A Taratuta<sup>1</sup>, K Jozsko<sup>1</sup>, B Gzik-Zroska<sup>1</sup>,  
R. Major<sup>2</sup>, A Dwyer<sup>3</sup>, M Dwyer<sup>4</sup>, Ł Mucha<sup>5</sup>, Ch Pfeifer<sup>6</sup>, M Fleisch<sup>7</sup>

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<sup>3</sup>CHIRSTOM Marcin i Marek Dwyer s.c., Poland

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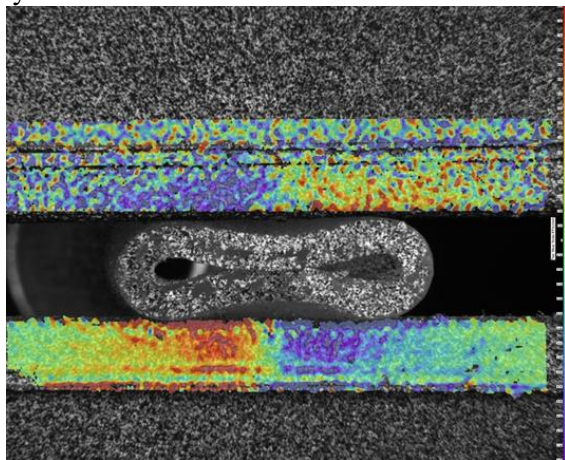
<sup>5</sup>Foundation of Cardiac Surgery Development, Institute of Heart Prostheses, Zabrze, Poland,

<sup>6</sup>DISTECH Disruptive Technologies GmbH, Austria

<sup>7</sup>Polymer Competence Center Leoben GmbH, Austria

## Abstract:

Th Vascular clamps are indispensable surgical instruments used to achieve temporary hemostasis during vascular procedures. However, despite being labeled as “atraumatic,” many existing designs still pose a risk of endothelial and vessel wall damage due to excessive or uneven clamping forces, unsuitable jaw geometry, and prolonged occlusion times. To reduce the tissue traumatization, some manufacturers offer so called atraumatic inserts made of soft materials; However, some studies show insufficient performance of the inserts mainly due to lack of reversible deformation to allowable limits. Therefore, the study included a numerical analysis of the newly developed tool with an insert made of metamaterials. taking into account the uniform pressure on the tissue. First, a geometric model of the tool was developed using CAD software. Then, a numerical model was developed. Appropriate boundary conditions were assumed for conducting the analysis - they reflected the phenomena occurring in the actual system.



**Figure 1:** Sample deformation map of tested insert models



**Figure 2.** Sample testing station

In the next stage of the work, the deformation of various variants of inserts made of metamaterial was assessed in order to verify the results obtained in the finite element analysis. The experimental tests were carried out using an MTS Insight 2 static testing machine and micro-correlation from Dantec Dynamic.

**Keywords:** atraumatic tools, minimally invasive surgery, innovative surgical tools, finite element methods, digital micro-correlation system

## Acknowledgments

The project was financed by the Polish National Center for Research and Development granted under the M-ERA.NET3/2022/75/AtraumaBioMat/2023 contract as part of the M-ERA.NET 3 Call 2022 competition; Austrian Federal Ministry – FFG grant number: FO999900377; Scientific and Technological Research Council of Türkiye: Tübitak Ardeb 1071 Programme grant number:123N419

## References:

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# Microparticle thermal conductivity measurements using Scanning Thermal Microscopy

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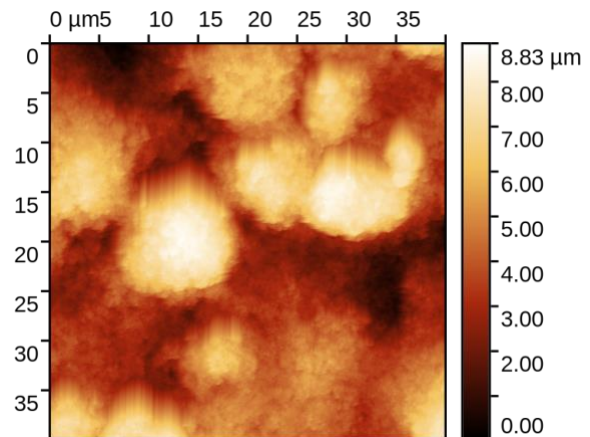
Department of Nanometrology, Czech Metrology Institute, Okružní 31, 638 00 Brno, Czech Republic

## Abstract:

Scanning Thermal Microscopy (S<sub>Th</sub>M) is a method belonging to Scanning Probe Microscopy family. S<sub>Th</sub>M uses a probe that can act as a heater and temperature sensor and therefore it can be used not only for topography measurement, but also for measurement of local thermal conductivity, by monitoring heat losses to the sample. As there are many parasitic heat flow paths in a typical S<sub>Th</sub>M experiment, quantitative values of thermal conductivity are typically obtained by calibrating the probe response on a set of bulk samples with known thermal conductivities. Microparticles such as lithium nickel manganese cobalt oxide (NMC) are frequently used in battery research and their thermal conductivity needs to be known to further enhance battery functionality. The shape of particles (see Fig. 1) however breaks the assumption used when calibrating the S<sub>Th</sub>M – samples are no more bulk.

In this contribution, we explore quantitative aspects of two potential approaches for particle thermal conductivity measurements using S<sub>Th</sub>M: using a set of spheres with known thermal conductivity, similar to the measured particle to calibrate the S<sub>Th</sub>M response and calibrating the S<sub>Th</sub>M on a set of bulk materials and fitting the measured data on a particle via a numerical model handling the geometrical differences between calibration samples and investigated particles.

**Keywords:** Scanning Thermal Microscopy, thermal conductivity, microparticles, lithium nickel manganese cobalt oxide, NMC, battery research, calibration, low carbon footprint battery.



**Figure 1:** Figure showing topography of battery cathode material with NMC particles embedded in carbon binder acquired with S<sub>Th</sub>M probe. The value of thermal conductivity of individual particle was evaluated from S<sub>Th</sub>M signal acquired on small area containing the given particle.



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