

Material Science at Large Scale Facilities (MSE-435): Case studies

Case study 1: Thermal fatigue in micro-electronics

Today, device manufacturers face the challenge of designing smart power devices tailored to meet the demanding requirements of emerging automotive applications. These devices need to conduct high power densities at rapid switching frequencies while maintaining a small footprint [1]. The small device dimensions result in elevated junction temperatures during short circuit events with strong current pulses as fast as 200 μs . At these timescales, heat dissipation via the packaging becomes ineffective, and in order to protect Si from thermal runaway, it is common to use $\sim 20 \mu\text{m}$ thick Cu metallizations to reduce operation temperatures [2]. However, previous investigations [3] have revealed that despite the thick metallizations, the ultra-short pulses can lead to peak temperatures of up to 350°C within the Cu. During the device's lifetime, multiple heating pulses may induce thermomechanical fatigue of the Cu metallization.

[1] D. Dibra, M. Stecher, S. Decker, A. Lindemann, J. Lutz, C. Kadow, On the Origin of Thermal Runaway in a Trench Power MOSFET, IEEE Trans. Electron Devices 58 (2011) 3477–3484. <https://doi.org/10.1109/TED.2011.2160867>.

[2] W. Robl, M. Melzl, B. Weidgans, R. Hofmann, M. Stecher, Last Metal Copper Metallization for Power Devices, IEEE Trans. Semicond. Manuf. 21 (2008) 358–362. <https://doi.org/10.1109/TSM.2008.2001210>.

[3] M. Nelhiebel, R. Illing, Th. Detzel, S. Wöhlert, B. Auer, S. Lanzerstorfer, M. Rogalli, W. Robl, S. Decker, J. Fugger, M. Ladurner, Effective and reliable heat management for power devices exposed to cyclic short overload pulses, Microelectron. Reliab. 53 (2013) 1745–1749. <https://doi.org/10.1016/j.microrel.2013.07.123>.



Case study 2: Kevlar yarns

Aramid yarns, often known by one of its trademark name Kevlar, are aromatic polyamids (poly-para-phenylene terephthalamide, PPTA) are high-performance synthetic yarns, which typically show high strength, high modulus and toughness. The multi-filament yarns are used for several applications such as structural reinforcement and bullet-resistant vests. Different mechanical properties can be achieved depending on processing conditions, see table 1 for four different commercial aramid yarns.

Description	Linear Density (g/1000 m) / nr of Filaments	Breaking Tenacity (mN/tex)	Modulus (GPa)	Elongation at Break (%)
low modulus	1680 f1000	2115	60	4.16
middle	1680 f1000	2350	91	3.45
high	1610 f1000	2135	105	2.7
ballistic	550 f500	2600	100	3.5

In the past, microscopy methods and X-ray techniques have been crucial to determine the presence of a complex fibrillar structure within the aramid fibers [1,2,3]. Studies indicate that the tensile properties of the filaments correlate with structural parameters within the fibers [3], the modulus being related to both micro-distortions (i.e. para-crystallinity) and structural orientation [2,3]. However more research is needed in terms of nano structure and its role in the materials properties, in particular towards properties such as the toughness which is an important property for ballistic applications. Another research interest is to investigate not only the yarn itself, but composite materials made with such yarns.

[1] Rao, Y., Waddon, A. J., & Farris, R. J. (2001). Structure-property relation in poly(p-phenylene terephthalamide) (PPTA) fibers. *Polymer*, 42(13), 5937–5946. [https://doi.org/10.1016/S0032-3861\(00\)00905-8](https://doi.org/10.1016/S0032-3861(00)00905-8)

[2] Pauw, B. R., Vigild, M. E., Mortensen, K., Andreasen, J. W., Klop, E. A., Breiby, D. W., & Bunk, O. (2010). Strain-induced internal fibrillation in looped aramid filaments. *Polymer*, 51(20), 4589–4598. <https://doi.org/10.1016/j.polymer.2010.07.045>

[3] Roenbeck, M. R., Cline, J., Wu, V., Afshari, M., Kellner, S., Martin, P., Londono, J. D., Clinger, L. E., Reichert, D., Lustig, S. R., & Strawhecker, K. E. (2019). Structure–property relationships of aramid fibers via X-ray scattering and atomic force microscopy. *Journal of Materials Science*, 54(8), 6668–6683. <https://doi.org/10.1007/s10853-018-03282-x>

Case study 3: High-density polyethylene (HDPE) under shear flow

High-density polyethylene (HDPE), a thermoplastic polymer, is commonly used in many packaging applications. The production process of choice is typically injection molding, where HDPE is melted at high temperatures and injected into a mold to create the required shape. HDPE is a semi-crystalline polymer which can form different morphologies, such as spherulites, where crystal chains extend radially from nucleation centers, elongated spherulites or shish-kebab microstructure [1]: extended crystal chains (shish) surrounded by folded lamellar crystals (kebab). An increased density of shish-kebab has been correlated with superior mechanical properties [2]. To optimize the process of injection molding in specific applications, it would therefore be interesting to different parameters to further understand these structure-property relationships and their dependence on these parameters [3].

[1] Odell, J. A., Grubb, D. T. & Keller, A. A new route to high modulus polyethylene by lamellar structures nucleated onto fibrous substrates with general implications for crystallization behavior. *Polymer* 19, 617–626 (1978).

[2] Keller, A., Kolnaar, H. W. H. Flow-induced orientation and structure formation. In *Processing of Polymers*. Vol. 18 (eds Meijer, H. E. H.) 189–268 (Wiley-VCH, New York, NY, USA, 1997).

[3] Mordal, K., Dobrakowski, K., & Kwiatkowski, D. (2018). Effect of Selected Injection Conditions on the Mechanical Properties and Structure of HDPE. In *Fibres and Textiles in Eastern Europe* (Vol. 26, Issue 5(131), pp. 93–98). Walter de Gruyter GmbH. <https://doi.org/10.5604/01.3001.0012.2538>



Case study 4: Extracellular matrix (ECM)

The extracellular matrix (ECM) is a complex network of macromolecules that provide structural and biochemical support to cells in the body. While it performs vital functions in the body, abnormalities in the ECM have been implicated to play an active or passive role in many pathological conditions, like cancer and fibrosis. The tumour microenvironment (TME) contains diverse ECM components that interact with cancer cells to facilitate tumour growth and metastasis [1]. The changing functional role of ECM in such cases manifests as a change in its structure [1, 2]. Furthermore, there is evidence of higher concentrations of certain elements as well as changes in their chemical forms, in certain cancers [3]. Therefore, a careful investigation into the composition and organization of the TME can help in a broad understanding of evolution of cancer and potentially identify biomarkers in specific cancer types.

- [1] Popova, N. V., & Jücker, M. (2022). The Functional Role of Extracellular Matrix Proteins in Cancer. In *Cancers* (Vol. 14, Issue 1, p. 238). MDPI AG. <https://doi.org/10.3390/cancers14010238>
- [2] Winkler, J., Abisoye-Ogunniyan, A., Metcalf, K. J., & Werb, Z. (2020). Concepts of extracellular matrix remodelling in tumour progression and metastasis. In *Nature Communications* (Vol. 11, Issue 1). Springer Science and Business Media LLC. <https://doi.org/10.1038/s41467-020-18794-x>
- [3] Sohrabi, M., Nikkhah, M., Sohrabi, M., Rezaee Farimani, A., Mirasgari Shahi, M., Ziaie, H., Shirmardi, S., Kohi, Z., Salehpour, D., Safarnezhad Tameshkel, F., Hajibaba, M., Zamani, F., Ajdarkosh, H., Sohrabi, M., & Gholami, A. (2021). Evaluating tissue levels of the eight trace elements and heavy metals among esophagus and gastric cancer patients: A comparison between cancerous and non-cancerous tissues. In *Journal of Trace Elements in Medicine and Biology* (Vol. 68, p. 126761). Elsevier BV. <https://doi.org/10.1016/j.jtemb.2021.126761>



Gallium nitride (GaN) is a highly promising material for use in light-emitting diodes, laser diodes, and high-temperature, high-power electronic devices. In particular, one-dimensional (1D) GaN nanowires (NW) have recently garnered significant interest within the field of materials science [1]. Research on GaN nanowires provides valuable insights into the fundamental properties of 1D systems and their potential applications in optoelectronic nanodevices. In particular, they have excellent mechanical properties, high thermal conductivity and interesting optical properties. The main sources of deterioration of NW's properties are their crystalline imperfection and residual strain. A better understanding of the relationship between some of these properties and internal microstructure is therefore crucial.

[1] A. P. Alivisatos, Science **271** (1996) 933

The cement industry is responsible for 7-8% of global CO₂ emissions per year, primarily because clinker production in Portland cement is an extremely energy-intensive process. Low-carbon cement (LCC) presents a sustainable alternative where the clinker content is reduced by using supplementary cementitious materials (SCMs) like fly ash, slag and calcined clay. Despite these obvious benefits, one hindrance is the poorly understood hydration kinetics and the changing nano/microstructure, especially in multicomponent systems. A thorough understanding of the mechanism of hydration and the structural evolution (both spatially and chemically resolved) that determine the properties of the LCC, will be a significant step forward.

[1] Winnefeld, F., Epifania, E., Montagnaro, F., & Gartner, E. M. (2019). Further studies of the hydration of MgO-hydromagnesite blends. In *Cement and Concrete Research* (Vol. 126, p. 105912). Elsevier BV. <https://doi.org/10.1016/j.cemconres.2019.105912>

Worldwide, an osteoporotic fracture occurs every 3 seconds and affects 1 in 3 women and 1 in 5 men over the age of 50. Diagnosis of osteoporosis is primarily based on areal bone density (aBMD) measured by dual energy X-ray absorptiometry (DXA). In fact, aBMD is a mediocre surrogate of bone strength and its sensitivity is limited by a large number of fractures not being diagnosed. It is now widely recognized that not just bone quantity, but also bone quality, which includes all geometric, compositional and architectural aspects of bone equally contribute to its strength and fracture risks [1,2]. Since bone is a highly complex and hierarchically structured material, it is important to understand the effect of this multi-scalar structure on the mechanical properties of bone.

[1] Osterhoff, G., Morgan, E. F., Shefelbine, S. J., Karim, L., McNamara, L. M., & Augat, P. (2016). Bone mechanical properties and changes with osteoporosis. In *Injury* (Vol. 47, pp. S11–S20). Elsevier BV. [https://doi.org/10.1016/s0020-1383\(16\)47003-8](https://doi.org/10.1016/s0020-1383(16)47003-8)

[2] Docaj, A., & Carriero, A. (2024). Bone health: Quality versus quantity. In *Journal of the Pediatric Orthopaedic Society of North America* (Vol. 7, p. 100054). Elsevier BV. <https://doi.org/10.1016/j.jposna.2024.100054>.



Case study 8: Nickel-based superalloys

Nickel-based superalloys are a key group of materials, especially in the growing areas of power generation and aerospace. These alloys have an impressive combination of properties, such as high strength and ductility at both room and high temperatures, as well as resistance to creep, fatigue, corrosion, and oxidation in challenging environments. They also have excellent thermal stability [1]. These properties result from their complex chemistry and structure, which usually includes solid solution strengthening, nano-sized γ' particles (mainly Ni_3Al with an L12 structure) in a face-centered cubic (FCC) γ matrix, and grain boundary strengthening from carbide phases. The γ' phase is particularly important for the strength of these alloys, as the interaction between the particles and the matrix leads to several strengthening mechanisms. Understanding how the material deforms and how this depends on features like the size and amount of γ' is crucial for developing models that can predict how the material will perform at high temperatures.

[1] R.C. Reed, The physical metallurgy of nickel and its alloys, Superalloys- Fundamentals Appl. (2006), pp. 33-120. DOI: 10.1017/CBO9780511541285

Case study 9: Pharmaceutical formulations

Controlled release drug delivery systems are designed to release therapeutic agents in a controlled manner over a prolonged period. Among these systems, polymer-based drug delivery mechanisms play a pivotal role. Phase-separated polymer systems consist of two or more immiscible polymers that form distinct microphases or domains within a drug-containing matrix. These domains influence the drug release profile, with different phases controlling the diffusion rate, matrix swelling, or erosion, which are critical in defining the drug release kinetics [1,2]. It is important to understand the structural and morphological changes that occur in phase-separated polymer matrices during dissolution and to investigate how phase separation, matrix degradation, and drug release kinetics are interrelated during the dissolution process.

- [1] Kamaly, N., Yameen, B., Wu, J., & Farokhzad, O. C. (2016). Degradable Controlled-Release Polymers and Polymeric Nanoparticles: Mechanisms of Controlling Drug Release. In *Chemical Reviews* (Vol. 116, Issue 4, pp. 2602–2663). American Chemical Society (ACS). <https://doi.org/10.1021/acs.chemrev.5b00346>
- [2] Yang, R., Zhang, G. G. Z., Zemlyanov, D. Y., Purohit, H. S., & Taylor, L. S. (2023). Release Mechanisms of Amorphous Solid Dispersions: Role of Drug-Polymer Phase Separation and Morphology. In *Journal of Pharmaceutical Sciences* (Vol. 112, Issue 1, pp. 304–317). Elsevier BV. <https://doi.org/10.1016/j.xphs.2022.10.021>

Case study 10: Iron mining for steel production

Iron is a critical raw material for steel production, and its extraction from ores such as hematite (Fe_2O_3) and magnetite (Fe_3O_4) forms the foundation of global industrial development. The extraction and processing of iron ore are influenced by a variety of factors, including the iron content, mineral composition, and the presence of impurities such as sulfur (S), phosphorus (P), and carbon (C) [1]. Additionally, valuable trace elements like chromium (Cr), nickel (Ni), and copper (Cu) may be present in ores, offering opportunities for secondary revenue streams. Exploring the quality of iron ores (composition as well as structure) using advanced large-scale facilities could offer valuable insights into their viability for industrial use.

[1] Park, J., Kim, E., Suh, I., & Lee, J. (2021). A Short Review of the Effect of Iron Ore Selection on Mineral Phases of Iron Ore Sinter. In *Minerals* (Vol. 12, Issue 1, p. 35). MDPI AG. <https://doi.org/10.3390/min12010035>

Lithium-ion batteries are an essential component of modern society due to their high energy density and long cycle life. They are widely used in portable electronics, such as smartphones and laptops, as well as in electric vehicles, renewable energy systems and large-scale energy storage systems. These batteries typically consist of a lithium-based cathode (such as LiCoO_2 , LiFePO_4 , or NMC—nickel, manganese, cobalt oxides), a graphite anode, and a liquid or solid electrolyte [1]. The continuous research into optimizing these components is essential to overcoming challenges like capacity degradation, thermal stability, and manufacturing costs. Additionally, the increasing demand for EVs and renewable energy storage is driving a need for more efficient, durable, and sustainable batteries. To achieve this, we need to investigate the battery's structure, chemical processes, and performance under real-world conditions, leading to breakthroughs in battery design and material science.

[1] Kim, T., Song, W., Son, D.-Y., Ono, L. K., & Qi, Y. (2019). Lithium-ion batteries: outlook on present, future, and hybridized technologies. In *Journal of Materials Chemistry A* (Vol. 7, Issue 7, pp. 2942–2964). Royal Society of Chemistry (RSC). <https://doi.org/10.1039/c8ta10513h>

The human brain is one of the most complex organs, responsible for cognition, motor control and emotions. Neurological disorders like Alzheimer's and Parkinson's disease have a far-reaching impact on the individual as well as societal level and yet the cause and mechanism of development of such disorders are poorly understood. The study of the brain's architecture at multiple scales and how they correlate is key to understanding both normal brain function and the development of neurological diseases [1]. It can also uncover insights into the neurochemical composition, neural pathways, synaptic functions and role of individual domains in specific disorders.

[1] Presigny, C., & Fallani, F. D. V. (2021). Multiscale modeling of brain network organization. arXiv. <https://doi.org/10.48550/ARXIV.2111.13473>

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