27 February 2025

PhD contract offer

Subject: Multiscale analysis of mechanical constitutive relations of polymers in relation to the evolution of their microstructure in real time.

General information

Workplace: Nancy, France
Type of contract: PhD contract
Contract period: 36 months
Expected date of employment: October 2025
Proportion of work: Full time
Remuneration: about 2200 € gross / month (minimum)
Required level of education: Master's degree in physics or material science.
Required experience: Internship and/or projects in at least one of the following fields: polymer science, solid mechanics, light-matter interactions physics.

Missions / Activities

Thermoplastic polymers are chosen for many structural applications because of their excellent mechanical properties and low density. Their use as a matrix in composites is also of great interest because of their versatility and recyclability. Understanding and being able to measure the changes that affect the microstructure of these materials when they are subjected to different thermal and/or mechanical loads is therefore crucial to controlling their shaping, in-service properties and durability. Among these thermoplastics, the polyester family includes many polymers that are widely used for their excellent mechanical and barrier properties, such as poly(ethylene terephthalate) (PET). Many polyesters are also interesting for their biodegradability (such as poly(lactic acid) (PLA)) and/or their bio-sourced origin (such as poly(ethylene furan-2,5-dicarboxylate) (PEF)).

For several years, the Physics, Mechanics and Plasticity team at the Jean Lamour Institute has been developing analysis methods that combine mechanical testing and in-situ analysis using Raman spectroscopy and X-ray diffraction (WAXS - Wide Angle X-ray Scattering). This work has made it possible to establish links between macroscopic mechanical behaviour and physical phenomena at the microstructural level (crystallinity, orientation of macromolecular chains, volume damage, mechanical load transfer, stress concentration, etc.) for several thermoplastic polymers and their composites [1-4], in particular PET [1-2] and PEF [3]. In this field, the last thesis defended in 2024 on this subject [5] highlighted two sets of results that will serve as a guideline for the subject presented here.

One of the results of this thesis, which extends the previous work of our team, shows the importance of monitoring the ester function in PET and PEF by Raman spectroscopy to quantify the order and hence crystallisation of these polymers [2-3]. The analyses tend to show that this correlation can be generalised to other polyesters. The first part of the thesis will therefore focus on consolidating the previous results and extending the analyses to other economically important polyesters, in particular PLA.
The second part of the thesis will focus on monitoring polymer deformation using Raman spectroscopy. The deformation of polymers involves a change in the organisation of the material at the macromolecular chain level, which is reflected, among other things, by the change in position of the measured vibrational bands. It has been shown that it is possible to quantify deformation by analysing Raman spectra recorded in situ during a mechanical test using the Grüneisen method [6-7]. In this way, our initial results for amorphous and semicrystalline PET and PEF in their glassy state indicate the possibility of calculating the evolution of the full strain tensor at the microstructural scale [5]. This work will therefore

focus on the application of this method to the polymers studied, in order to confirm and improve our preliminary results and provide a better understanding of their properties.

This work will include a significant experimental component. This will be based on mechanical tests coupled with in situ Raman spectroscopy measurements. These Raman measurements will also be complemented and validated by in situ WAXS tests performed on large scientific instruments (such as the synchrotrons ESRF in Grenoble or Alba in Barcelona), which are a speciality of the host team. This topic also involves a lot of results analysis and signal processing. Good programming skills (Python/MATLAB) are therefore appreciated. Depending on the progress of the work, it may be possible to apply the results obtained to the development of mechanical constitutive models for polymers that take into account physical phenomena at the microstructural scale.

References

[1] M. Donnay, M. Ponçot, J-P Tinnes, T. Schenk, O. Ferry, I. Royaud, "In situ study of the tensile deformation micro-mechanisms of semi-crystalline poly(ethylene terephthalate) films using synchrotron radiation x-ray scattering". Polymer, 117, 268–281, (2017).
[2] M. Bouita, J.P. Tinnes, P. Bourson, M. Malfois, M. Ponçot, "A new Raman spectroscopy-based method for monitoring the crystallinity ratio of polyethylene terephthalate". Journal of Raman Spectroscopy, 54 (2), 225-232, (2023).
[3] M. Bouita, J.P. Tinnes, P. Bourson, M. Ponçot, "Monitoring The Thermal Behavior of Polyethylene 2,5 Furandicarboxylate Using Raman Spectroscopy". Journal of Raman Spectroscopy, 54 (6), 683-690, (2023).
[4] M. Ponçot, J. Martin, S. Chaudemanche, O. Ferry, T. Schenk, J.P. Tinnes, D. Chapron, I. Royaud, A. Dahoun, P. Bourson "Complementarities of high energy WAXS and Raman spectroscopy measurements to study the crystalline phase orientation in polypropylene blends during tensile test", Polymer, 80, 27–37, (2015)
[5] M. Bouita, "Étude des propriétés et des lois de comportement mécaniques à différentes échelles de polyesters par WAXS et spectroscopie Raman in situ", Thèse de Doctorat, Université de Lorraine (2024)
[6] B.D. Sanditov, S. Sh. Sangadiev, D. S. Sanditov, "Gruneisen parameter and fluctuation volume of amorphous polymers and glass", Glass Physics and Chemistry, 39, 382–389, (2013).
[7] R. J. Young, "Raman spectroscopy and mechanical properties", In: Spells S.J. (eds): Characterization of Solid Polymers. Springer, Dordrecht, (1994).

Keywords

Polymers, Mechanics, Microstructure, Raman spectroscopy, X-rays diffraction

Work context

The PhD student will work under the supervision of Dr. Marc Ponçot and Dr. Jean-Philippe Tinnes within the Physics, Mechanics and Plasticity research group of the Institut Jean Lamour, at the main laboratory's site (Artem) in Nancy, France.

Skills

- Must hold a Master's degree in Materials Science or equivalent.
- Knowledge in polymers physics and mechanics. Some competencies in one of the following subjects will be appreciated: Raman spectroscopy, X-ray diffraction, crystallography.
- Proficiency in programming and data treatment (Python / MATLAB)
- English fluency

About Institut Jean Lamour

The Institute Jean Lamour (IJL) is a joint research unit of CNRS and Université de Lorraine.
Focused on materials and processes science and engineering, it covers: materials, metallurgy, plasmas, surfaces, nanomaterials and electronics.
It regroups 183 researchers/lecturers, 91 engineers/technicians/administrative staff, 150 doctoral students and 25 post-doctoral fellows.

Partnerships exist with 150 companies and our research groups collaborate with more than 30 countries throughout the world.
Its exceptional instrumental platforms are spread over 4 sites; the main one is located on Artem campus in Nancy.

Application

Applicants are invited to send a CV and cover letter to:
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