INTERNSHIP PROPOSAL

(One page maximum)

Laboratory name: Institut Charles Sadron
CNRS identification code: UPR22
Internship director'surname: PECORA and FALL
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Internship location: Institut Charles Sadron (Strasbourg)

Thesis possibility after internship: Opportunity to participate in the doctoral school audition
Funding: YES Laboratory funding

Molecular Dynamics Simulation of Pre-Oriented Polymers

Context

Polymer processing often involves large deformations that align macromolecular chains in the amorphous phase, which makes the resulting material anisotropic and direction-dependent. Recent experimental studies at the Institut Charles Sadron focused on pre-oriented polycarbonate (PC), a high-performance transparent thermoplastic commonly used in applications such as eyeglass lenses and aircraft windscreens. In these experiments, samples were stretched up to a ratio of about 1.7 and then tested mechanically at different angles relative to the orientation direction. The results revealed contrasting behaviors: while yield stress and strain hardening increased with angle in compression, they decreased in tension. Moreover, indentation and scratch tests showed a preferential pile-up normal to the drawing direction, which appeared inconsistent with the bulk compressive response. These findings highlight a strong tension–compression asymmetry that is amplified by orientation, raising open questions about the multiscale origins of this behavior. Understanding the molecular level origin of the anisotropic response to indentation could lead to PC plastics with autonomous self-healing properties.

Objectives

The objectives of the internship are as follows:

1. Implement classical molecular dynamics in LAMMPS, with a coarse-grained model polymer model, to create amorphous (disordered) and pre-oriented (aligned) PC-like samples by pre-stretching.
2. Deform the simulation cell uniaxially in all-directions (x,y,z) to mimic mechanical tests and plastic drawing of both amorphous and pre-oriented PC samples.
3. Extract components of the pressure tensor (strain), quantify entanglements between polymer chains and local nematic ordering to determine if a correlation exists between them and compare with experiments. Such topological features cannot currently be quantified experimentally during mechanical testing.
4. Time permitting, implement nanoindentation simulations to mimic anisotropic pile up and determine its molecular origins in pre-oriented vs amorphous samples.

Candidate Profile

Masters or final-year engineering student in physics, materials science, or physical chemistry with an interest in molecular simulations, polymer physics or mechanics. Candidates should have a firm grasp of statistical physics. Candidates with existing experience with molecular simulations (LAMMPS), HPC clusters of the CNRS (Adastra/Jean-Zay) and programming (Python/C/C++) are highly sought after.

Please, indicate which speciality(ies) seem(s) to be more adapted to the subject:

Condensed Matter Physics:	YES	Soft Matter and Biological Physics:	YES
Quantum Physics:	NO	Theoretical Physics:	YES