CONFORMATION CONTROL OF CHIRAL MOLECULES IN AN ELASTOMER UNDER MECHANICAL STRETCHING: MATERIAL ORGANIZATION STUDY BY POLARIMETRY

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KEYWORD(S) : Polarimetry / Spectroscopy / Soft mechano-chemistry

SCIENTIFIC CONTEXT :

This project is a part of the ELASTIxMOL ANR granted project which aims at tuning the 3D geometry of chiral molecules grafted in elastomer by applying a macroscopic unidirectional force, in a continuous and reversible way. The understanding of the underlying mechanisms of this soft-mechanochemistry process will open the way toward the developments of smart materials where by a simple mechanical action the material properties can be tuned in a reversible way. The objective of this thesis is to study the chiroptical response of the molecular deformation of chiral molecules under stretching of the elastomers they are grafted to.

The main challenge will be to extract the differential chiral signals from the differential linear effects that are order of magnitude more intense. Indeed, our preliminary work (figure) shows that under stretching the polymer chains unfold and align themselves. This modifies not only the chiroptical responses of the chiral molecules but also induces linear contributions that are much higher (x1000) than the chiral ones. They then mix together to give false, difficult to predict, chiroptical signals. By investigating specially designed mechano-sensitive chiral molecule series, we want to address the ability of soft-mechanochemistry to manipulate molecular conformation through the stretching of a 3D elastomer

MISSIONS :

The first objective of this thesis will be to optimize the whole process by angular orientation automation and force measurement. A thorough full Stokes/Mueller analysis will be conducted in order to extract the chiroptical tensor of the molecules as a function of the stretching ratio. The use of a new molecule series with allowed transitions in the spectral window of the PDMS will allow the access to strong chiral signals. Moreover, the study of samples with different material properties, will offer the unique ability to investigate the interplay between circular and linear effects that are sources of many artifacts and misinterpretations. The second objective is the development of chiral luminescence detection and again finding the way to overcome signal contributions coming from linear effects. The main advantages will be the wavelength detection shift (Stokes shift) and the possibility to perform chiral mapping of the stretched objects. Finally, by relating the conformational change of a given chiral molecules/PDMS host association to the mechanical stretching force, we will end up with a clear understanding of the underlying soft-mechanochemistry process.

OUTLOOKS :

Academic or indusrial research

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