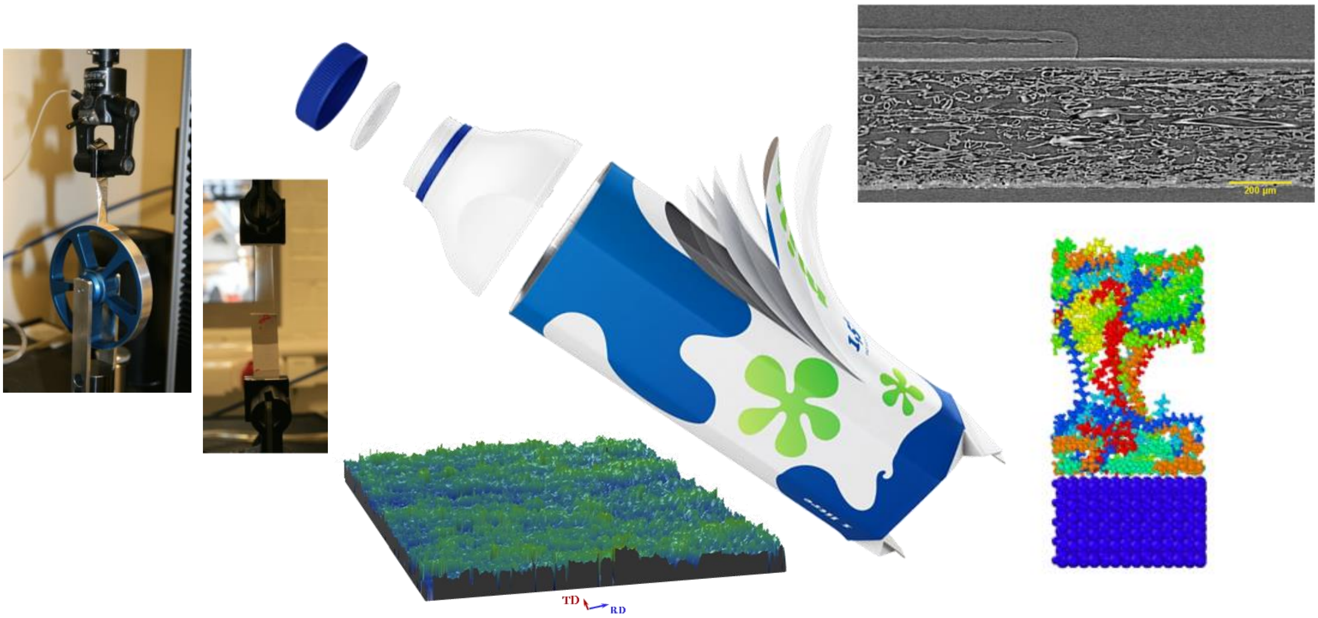
MULTISCALE MODELING OF ADHESION MECHANISMS

Master Thesis Proposal

Packaging material is a laminated composite structure consisting of several different layers. Each layer is needed with its specific functionality e.g. provide stability of the package and to provide an oxygen barrier for the filling product. Furthermore, the surface interfaces of the layers must also adhere - ‘stick together’.

Adhesion is a complex phenomenon and must be described using multiple length scales. At the atomistic level, chemical bonds between functional groups on the surfaces are present. On the microscopic level, small defects and irregularities may occur, and finally, on the macroscopic level the material is stressed by outside factors, e.g. a consumer dropping a package on the floor.



In recent work, investigations of adhesion mechanics have been carried out on the atomistic scale using density functional theory and molecular dynamics[1], and also on the micromechanical scale using both X-ray imaging and mathematical modeling[2]. The purpose of this master thesis project is to start linking the atomistic and microscale together using a multi-scale modeling approach.

In more detail the thesis would include

- Literature study of multiscale modeling methods and techniques
- Establish what simulation methods are relevant for this specific application
- Investigate if peridynamics[3] modeling could be applied
- Suggestion of workflow to set up a multiscale modelling framework

The work will be carried out at Tetra Pak in Lund in collaboration with the Department of Mechanical engineering Sciences, Division of Mechanics at Lund Institute of Technology.

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References

1 Olsson, et al. (2020) Atomistic investigation of functionalized polyethylene-alumina interfacial strength and tensile behaviour, Computational Materials Science, https://www.sciencedirect.com/science/article/pii/S0927025620305668

2 Pettersson, et al., (2019) Peel testing of a packaging material laminate studied by in-situ X-ray tomography and cohesive zone modeling, International Journal of Adhesion and Adhesives, Volume 95, https://www.sciencedirect.com/science/article/pii/S0143749619301691

3 Ahadi, et al (2018) Capturing nanoscale effects by peridynamics, Mechanics of Advanced Materials and Structures. 25, 13, p. 1115-1120