Public summary of PhD-thesis of Christos Mitrias
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Computational tools that reduce the cost and accelerate the development process of foams and blends

Foams and blends are everywhere around us because of their versatility. Their microstructure determines their characteristics, for example how they absorb impact or sound, or how well they insulate. To better study these materials, Christos Mitrias developed computational tools that focus on the behaviour of the interfaces between the components of the mixture, as those interfaces are crucial for the material properties. These tools save time in materials development and are applicable in a broad range of applications.

Better materials can be created by developing new molecules. However, a quicker and cheaper method is to physically blend already existing materials that are immiscible. One of the reasons that blends show different properties than their constituents is because of the presence of interfaces between the individual components. Choosing the right materials to mix is essential to produce blends with enhanced properties. In particular, polymer foams are becoming increasingly important materials in the industry; they are light and strong and during processing there is a great deal of freedom to create almost any desired shape. Foams are two-phase materials which show an internal cellular structure, similar to natural materials like sponges, cork, balsa wood and trabecular bone. These materials show advanced properties, such as sound and energy absorption that depend on their microstructure. Apart from the improved properties that cellular materials exert, they can also contribute to energy saving due to their lightweight structure.

Nevertheless, finding the proper materials to blend and the right processing conditions can be challenging and requires performing several costly experiments. That is why developing computational tools to perform simulations instead can be very useful. By performing the appropriate simulations, the number of experiments needed can be substantially reduced. Furthermore, using a multiscale framework it is possible to obtain essential parameters from different scales and thus give a greater physical insight.

In this thesis, we present several computational tools that can be used to study the material properties of blended materials with fluid-fluid interfaces (which also includes gas-liquid interfaces). There are two main classes of methods for the modelling of fluid-fluid interfaces, where there is either a sharp transition between the two materials or a finite distance in which the change from one material to the other occurs. Our choice of preference in this thesis is the former since this type of methods allows for a much more accurate representation of the geometric features. Novel computational methods were developed that provide a great insight into the effect that the presence of interfaces has on such materials in an efficient and robust way. Some examples are the study of the film drainage between two drops that collide in a blend and the prediction of the final microstructure of a foam which plays a significant role on the final material properties.

Although the application in this thesis was focused mainly on blends and foams, all the tools have been derived in a generic way making it possible to employ them in a broader range of applications.

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