

# YIELDING OF PHASE CHANGE MATERIALS TO HEAT AND/OR STRESS: THE PHASE TRANSITIONS PICTURE

GIORGIA FUGALLO, MIGUEL MOYERS-GONZALEZ, TEODOR BURGHELEA

Pasty materials are relevant to a number of practical applications related to several modern industrial sectors including (but not limited to) food industry, polymer processing, pharmaceuticals, cosmetics, petroleum etc. In the absence of external forcing (temperature and/or stress) they behave as solids (they do not flow though they may sustain some finite external forcing) but, if the external forcing exceeds a certain threshold, their micro-structural integrity is lost and exhibit a liquid behavior (they flow). Depending on their molecular structure, this solid-fluid transition may be triggered by two distinct types of external forcing: heating or stressing. In the specific case of phase change material (PCM) they undergo a solid-liquid transition while being heated [1] while physical gels yield to stress while gradually sheared, [2]. While it is rather clear that the solid-fluid transition is associated to micro-structural changes triggered by either the temperature or the applied stress, the exact physical scenario and the microscopic picture of the yielding process remain elusive. As the yielding to stress is concerned, the vast majority of previous studies propose macroscopic phenomenological models that are merely mimicking a change from a solid like rheological behavior (often Hookean) to a shear thinning fluid behavior, Ref. [3, 4, 5, 2]. While clearly useful from an engineering standpoint, such models are physically unsatisfactory (to be blunt, some of these models are inconsistent with the second law of thermodynamics!). It was recently suggested that a physically sound framework for understanding the solid-liquid transition in pasty materials subjected to an external stress is that of phase transitions and critical phenomena [6, 7, 8]. The main scope of the proposed project is to extend the initial studies reported in Refs. [6, 7, 8] using state of art molecular dynamics simulations [9]. This approach will cover both the case of the yielding to stress and the case of the yielding to heat. Several key aspects will receive a particular attention through the project. First, how is the dynamics of the solid-fluid transition affected by the level of interaction between the microscopic constituents? Is the yielding scenario of a neutral gel (such as agar gel) mainly formed by hydrogen bonds similar to that of a strongly attractive colloidal gel (such as bentonite, laponite). Next, when the material is gradually forced (or, in an engineering jargon, "*loaded*") how does the physical nature of the solid-fluid transition (first, second order- thus we are mainly questioning its reversibility) relate to the degree of steadiness of the forcing? How comparable is the case of quasi-steady forcing to the case of very fast forcing? Similar questions will be addressed for the case of the yielding to heat (in the presence or absence of a mechanical stress field).

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The PhD project will be carried on in two stages. For the first 18 months, the candidate will work at LTeN Nantes under the supervision of Dr. Giorgia Fugallo and Dr. Teo Burghlelea on implementing state of art molecular dynamics simulations for the yielding of a pasty material. Based on a statistical analysis of these results, novel constitutive relationships for yield stress materials will be derived. The second half of the thesis will be spent in the School of Mathematics and Statistics at University of Canterbury, NZ, under the supervision of A/Prof. Miguel Moyers-Gonzalez. In this part of the project, the new constitutive relations will be put to the test in numerical simulations for relevant industrial flows.

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