M2 INTERNSHIP PROPOSAL

Probing the Molecular Mechanism of 'Melting on Cooling' in Polyphosphazenes with Molecular Simulations

Laboratory: [a]Institut Charles Sadron, Université de Strasbourg & CNRS, Strasbourg, France. [b]Institute of Materials Chemistry, School of Materials Science and Engineering, Xi'an Jiaotong University, PR China.

Supervisors: [a]William Fall (william.fall@ics-cnrs.unistra.fr) & [b]Goran Ungar (g.ungar@xjtu.edu.cn)

Proposal: Gustav Tamman first acknowledged the possibility of crystal melting on cooling in 1902 **[1]**. The first experimental examples however were not discovered until the 1990s in poly-4-methylpentene, a polymer which, like ice, shrinks on melting **[2]**. We now want to study a different polymer, known as Polyphosphazene, which in addition to melting on heating, exhibits a mesophase which melts on cooling **[3]**. The aim is to understand the molecular mechanism behind melting on cooling, using molecular dynamics simulations of model branched polymers. The results could provide new understanding of entropy-driven phase transitions. Melting on cooling is useful because it allows materials to absorb heat and regulate temperature, store and release energy efficiently, and sometimes flow or self-heal at low temperatures, making it valuable in thermal management and certain mechanical applications. For instance, if glass-forming or semi-crystalline polymers at low temperature need to remain soft, they could be blended into composites with Polyphosphazene.

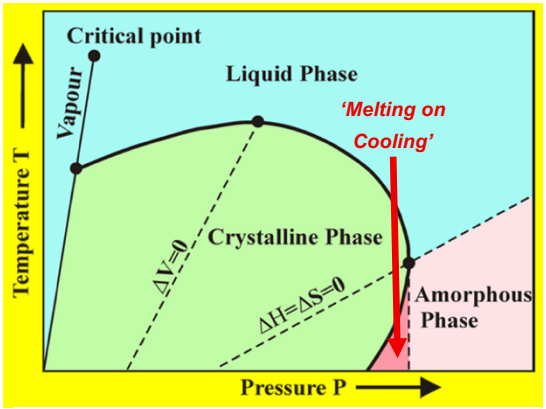

Fig 1 *– Tammann's Universal Pressure and Temperature Phase Diagram.*

Objectives: **(1)** Implement classical molecular dynamics, with a model polymer force-field, to grow the mesophase. **(2)** Identify key force-field parameters and capture melting on cooling in simulations. **(3)** Time permitting understand the influence of side chain length on the transition temperature and compare with experiment.

Candidate Profile: Masters or final-year engineering student in physics, materials science, or physical chemistry with an interest in MD simulations and polymer physics. Existing experience with molecular simulations (LAMMPS), HPC clusters and programming (Python/C/C++) are highly sought after. The internship will be based at the Institut Charles Sadron in Strasbourg, with the earliest start date in February, to allow sufficient time to acquire authorization from the Ministry of Defence. Candidates requiring a visa should anticipate an additional 1-2 months before starting and ensure the starting date and project duration (6 months) fits the curriculum/defence date set by their host institution. Applications, including a CV and covering letter, should be sent to: william.fall@ics-cnrs.unistra.fr.

References: **[1]** Tammann, G., Kristallisieren und Schmelzen. Johann Ambrosius Barth, Leipzig, 1903. **[2]** Rastogi, S., Pressure-induced amorphization and disordering on cooling in a crystalline polymer. *Nature,* 1991. **[3]** Papkov, V. S., et al. Unusual phase behaviour of some poly dialkoxyphosphazenes. *Macromolecules,* 1992.

Institut Charles Sadron | CNRS | UPR22
23 rue du Loess
67034 Strasbourg Cedex 2
Tél. +33 (0)3 88 41 40 00
Fax. +33 (0)3 88 41 40 99
www.ics-cnrs.unistra.fr