RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Materials Science, Mechanics, Fluids

Subfield: Applied Physics, Structure Design, Organic & hybrids Materials

Title: Digital Crystallization of Organic-based systems: from Spherulites to Dendrites

ParisTech School: MINES ParisTech | PSL

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**2MS team: https://www.cemef.minesparis.psl.eu/en/presentation/team-2ms/*
***CFL team: https://www.cemef.minesparis.psl.eu/en/presentation/team-cfl/*
****BIO team: https://www.cemef.minesparis.psl.eu/en/presentation/team-bio/*

Short description of possible research topics for a PhD:
The physics of the growth kinetics (GK) of polymer structures is lagging behind in certain points compared to that developed in metallurgy [1-3]. Indeed, if numerical model of the GK of structures (e.g., dendrite, eutectic) is a major research topics in physical metallurgy since decades [3], the theories of polymer GK remain rare [1,2].
To address this scientific barrier, in this thesis proposal, polymer & metal cross-fertilization is highlighted (**Figure 1**). Phase field methods will be developed to **i-** give a description of growth and a criterion of transition between spherulitic and dendritic crystals in accordance with the experiments carried out on carefully selected model organic systems (**b** & **c**), **ii-** identify the phase diagram of systems and correlate it to microstructural evolutions (**d**), and **iii-** integrate a new thermodynamic parameter including the effect of pressure (CRISTAPRESS cell, etc.) [4].

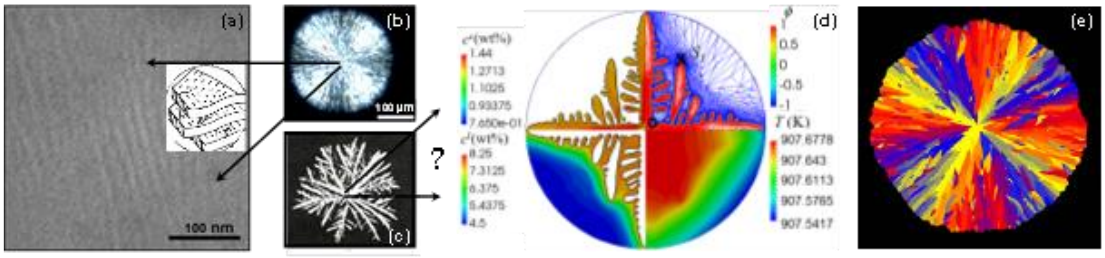

Figure 1 **(a)** Crystalline lamellae (nano), **(b)** spherulite (micro) (iPP, *Boyer*, MINESParis PSL); **(c)** branches of dendrites in polymer mixtures (iPP/aPP, *Keith & Padden*); phase field simulation of **(d)** dendritic growth (*Sarkis*, MINESParis PSL thesis [3]), **(e)** polycrystalline spherulitic growth (*Gránásy* [DOI: 10.1103/PhysRevE.72.011605]

Fallout

- New breakthrough in crystallization of organic systems
- Physics based on model polymer systems (petro-sourced, bio-sourced) [1,5]

- Development of numerical and experimental methods
- Thermodynamic/kinetic coupling (diffusion of energy and species) & structure
- Application to other morphologies (transcrystalline structure, foam, multi-transformations design, etc.) [1,5]

Required background of the student:
Main fields required are in Computational Mechanics and Materials Science.
The applicant will be involved in digital and experimental works.

A list of 5 (max.) representative publications of the group:

1. S.A.E. Boyer, J.-P.E. Grolier, H. Yoshida, J.-M. Haudin, J.-L. Chenot, "*Thermodynamic and Thermokinetics to model phase transitions of polymers over extended temperature and pressure ranges under various hydrostatic fluids*" in "Thermodynamics-Interactions Studies-Solids, Liquids and Gases", J.C. Moreno-Pirajan (Ed.), 2011. DOI: 10.5772/24402 - J.-M. Haudin, S.A.E. Boyer, *"Crystallization of Polymers in Processing Conditions: An Overview"*. International Polymer Processing, 32: 545-554, 2017. DOI: 10.3139/217.3415
2. D. Hoffman, R.L. Miller, *"*Kinetic of crystallization from the melt and chain folding in polyethylene fractions revisited: theory and experiment*"*. Polymer, 38: 3151-3212, 1997. DOI: 10.1016/S0032-3861(97)00071-2
3. C. Sarkis, "Modélisation de la solidification dendritique d'un alliage Al-4.5%pdsCu atomisé avec une méthode de champs de phase anisotrope adaptative". PhD thesis *MINESParisTech CEMEF, 2016*
4. S.A.E. Boyer, F.E.J Fournier, Ch.-A. Gandin, J.-M. Haudin, *"CRISTAPRESS: An optical cell for structure development in high-pressure crystallization"*. Review of Scientific Instruments, 85: 013906 1-8, 2014. DOI: 10.1063/1.486(2473-6646)
5. S.A.E. Boyer, J.-Marc Haudin, V. Song, V. Bourassier, P. Navard, C. Barron. *"*Transcrystallinity in maize tissues/polypropylene composites: First focus of the heterogeneous nucleation and growth stages versus tissue type*"*. Polymer Crystallization, Wiley, In press, DOI: 10.1002/pcr2.10155