French Polytech network form for PhD Research Grants from the China Scholarship Council

This document describes one of the PhD subjects proposed by the French Polytech network. The network is composed of engineering schools/universities. The document also provides information about the supervisor.

Supervisor information	
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PhD information	
Title	Phase Change Kinetics under Supercooling during Partial Thermal Cycles: A Molecular Dynamics Approach
Main topics regards to CSC list (3 topics at maximum)	IV-1. Nanotechnologie et Nanotechnique (Nanotechnology and Nanotechnique) IV-2. Nanomatériaux (Nanomaterials) IV-11. Matériaux d'information, de stockage et de capteurs (Information, storage and sensor materials)

Required skills in science and engineering	Materials science, physics and chemistry of materials, thermodynamics and chemistry of phase change materials, with particular expertise in molecular dynamics simulations and proficiency in programming languages

Subject description (two pages maximum including biblio)

Phase change materials (PCMs) are key components of thermal energy storage systems, widely used in buildings, electronics cooling, and district heating networks [1, 2]. However, their real-world behavior often departs from standard characterization methods with constant transformation rate (DSC), particularly when subjected to partial melting and solidification cycles, and/or as a recalescence phase is observed with a high volume of supercooled PCM. These conditions induce variable transformation rates, thermal hysteresis, and memory effects that remain poorly understood at the atomic scale.

The proposed research aims to explore out-of-equilibrium phase transformations using molecular dynamics (MD) simulations, an approach already widely applied to various material matrices [3–6]. The objective is to better understand the atomic-scale mechanisms governing these transitions under realistic thermal loads. The conceptual framework will rely on established recommendations for analyzing complex multi-step kinetic processes, notably those from the ICTAC kinetics committee, which will guide the simulation methodology.

Several PCMs known for their supercooling behavior will be studied. Sodium acetate trihydrate, for example, has recently been analyzed experimentally and by MD, highlighting local structural factors influencing crystallization nucleation [7]. $Na_2HPO_4 \cdot 12H_2O$ exhibits strong thermal hysteresis and has also been studied via MD [8], while $Na_2SO_4 \cdot 10H_2O$ has been used to investigate atomic-scale conditions delaying nucleation [9]. In parallel, certain metals such as silver provide complementary model systems where the role of supercooling and crystallographic orientation on front propagation velocity can be more easily isolated [10]. Recent work has also addressed challenges related to the precise determination of melting temperature by MD, evaluating the efficiency and robustness of various approaches [11].

More generally, the use of MD for PCMs is rapidly expanding, with reviews emphasizing the importance of linking atomic behavior to macroscopic performance [12]. Some studies even propose extending this connection to phonon physics to explain thermal performance under cyclic conditions [13]. Others review strategies aimed at enhancing the thermal properties of PCMs, stressing the fundamental role of atomic-level understanding of phase transitions [14].

The methodology of this thesis will be based on MD simulations under controlled thermal ramps (heating and cooling), allowing observation of nucleation, growth, and regression of the solid-liquid interface during partial cycles for PCMs exhibiting phase change hysteresis. Particular attention will be paid to designing realistic thermal cycles to extract kinetic laws that can be used in multiscale models. This work is expected to improve our understanding of transient phase change dynamics and provide predictive models integrable into thermal system simulations, while proposing atomic-scale criteria for the design of next-generation PCMs with enhanced performance and reliability.

References:

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