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Editorial

Structural transformations and non-equilibrium phenomena in multicomponent disordered systems

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Abstract The issue is devoted to theoretical, computational, and experimental studies of phase and structural transitions and non-equilibrium phenomena (phase transformations, heat generation, rheology, and relaxation phenomena) in disordered systems, e.g., composite and metastable materials, biological tissues and systems; polymer and other soft materials; amorphous and glass-forming systems, as well as multicomponent melts. Special attention is paid to the detailed microscopical study of various phenomena in the aforementioned systems.

1 Introduction

The present issue covers the rapidly developing research area of multicomponent materials with complex disordered internal structures (Fig. 1). It includes multiple disciplines ranging from the non-equilibrium statistical physics of microscopic effects to phenomenological non-equilibrium thermodynamics, condensed matter physics, and biomedical applications.

To represent a complex picture of micro- (nano-) and meso-temporal and spatial scales in phase- and other non-equilibrium phenomena, a study of various heterogeneous materials (from metastable and multicomponent liquids to biological cell cultures) is included. Special attention is paid to developing the scientific background for biomedical applications, such as the intensification of addressing drug delivery in thrombosed blood vessels, Rab5/Rab7 protein dynamics and escape of pH-sensitive nanoparticles and viruses from endosomes, magnetic hyperthermia as a method of cancer therapy, hemodynamics in branched coronary arteries, as well as non-contact diagnoses of stenosis.

2 The general content of the issue

New aspects of structural transformations appearing in metastable and non-equilibrium liquids as a result of directional and bulk crystallization processes are discussed in Refs. [1–10].

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Namely, a linear analysis of morphological stability of a planar solid–liquid interface in the presence of melt convection is studied in Ref. [1], where both cases of slow and intense convection described by conductive and convective heat and mass transfer boundary conditions are considered. When dealing with conductive boundary conditions, two various crystallization regimes with mushy and slurry layers developing ahead of the crystallization front may occur. When dealing with purely convective boundary conditions, the crystallization process is stable.

The linear and non-linear theories of dynamic instability of steady-state crystallization with a mushy layer are developed in Refs. [2, 3]. In Ref. [2], the authors demonstrate the possibility of an oscillatory mode of instability development using a linear analysis. Then, they describe the impurity layered liquidation in solids using a non-linear analysis in Ref. [3].

Linear morphological stability of the planar interface in the moving melt is studied in Ref. [4] with allowance for the plane-parallel flow of one liquid relative to another one. Here, the stationary solution, dispersion relation, and neutral stability surface are obtained using boundary integral theory. This theory was also used in Ref. [5] to highlight that the melt undercooling at the dendritic surface can change about 5–7% in the presence of a small flow slope.

In Ref. [6], based on a mushy layer model and stochastic analysis, the authors show that sea ice freezes faster when fluctuations in the atmospheric temperature and friction velocity occur. Directional crystallization with a mushy layer, when the melt convection plays an important role, is analytically described and compared with

Fig. 1 Dendritic ice crystals (Lake Tavatui, Sverdlovsk Oblast, Russia)

experiments in Ref. [7]. How constitutional supercooling influences the mushy layer origination is described in Ref. [8].

Analytical theory of purely bulk crystallization with spherical particles at the intermediate stage of phase transitions is considered in Ref. [9]. Using the saddle-point technique, the authors found the crystal-radius distribution function and the law of metastability reduction. How the shape of evolving crystals influences the evolution of particulate assemblages in supercooled and supersaturated liquids is summarized in a review article [10].

The effects of mass influx and withdrawal of product crystals on the evolution of crystal assemblages in a crystallizer are analyzed in Ref. [11]. Unsteady, steady, and self-oscillatory modes of the bulk continuous crystallization are described analytically. The applications of structural transformations in non-equilibrium phenomena of particle transport in blood vessels and living cells are studied in Refs. [12] and [13]. Namely, a mathematical model of magnetic nanoparticles transport in a channel modeling a blood vessel with stenosis is introduced in Ref. [12]. The obtained results of computational simulations reveal the presence of stagnant zones with vortices of the host liquid that appear near the stenosis. An increased concentration of magnetic nanoparticles near the stenosis makes it possible to determine the position and size of the stenosis using an external magnetic sensor. A stochastic model of the conversion of early endosomes into late endosomes involving the replacement of Rab5 by Rab7 protein levels is studied in Ref. [13]. Numerical simulations show that Rab5 experiences a quicker initial growth compared with Rab7, but the latter eventually surpasses Rab5 and becomes dominant with strong random fluctuations. This process leads to a random decrease in endosomal pH and, as a consequence, the random escape of pH-sensitive nanoparticles and viruses from the endosomes. Reference [14] proposes physico-mathematical models for cavitation of microbubble clouds under the influence of bubble-bubble interaction during histotripsy. The mathematical models are formulated for non-interacting and inter-particle interacting microbubble clouds on histotripsy considering the effect of variable surface tension.

In Ref. [15], structural transformations in coupled multicomponent biological systems are considered. It is shown that, due to these transformations, the synchronization type changes and transitions from order to chaos can occur. In Ref. [16], it is shown that calcium oscillations, playing a key role in cellular processes, are deformed by random noise. Parametric analysis of stochastic transformations of calcium relaxation self-oscillations is carried out using statistics extracted from the direct modeling and a new theoretical approach based on the method of confidence domains.

Reference [17] studies the effect of convective flow on primary dendrite spacing between neighboring crystals within a dendrite ensemble. Solidification of a binary alloy is considered within the model of a stagnant boundary layer under an imposed thermal gradient that influences the crystal microstructure and chemical microsegregation. In Ref. [18], the tip shape function is analyzed and tested against experimental data and numerical simulations when external impacts such as forced convection and dissolved impurities play a decisive role. In Ref. [19], the microstructures of Al-12.6 wt.%Si–0.8 wt.%Mg–0.4 wt.%Mn–0.7 wt.%Fe–0.9 wt.%Ni–1.8 wt.%Cu are obtained by rapid quenching. A mechanism for the layered microstructure formation, which considerably changes the material properties, is proposed in Ref. [19].

Nanodisperse soft and liquid magnetic composites (ferrogels, ferrofluids) are materials consisting of either polymer or liquid host media with embedded colloidally stabilized single-domain ferro/ferrimagnetic particles. These systems attract substantial interest of researchers, engineers, and bio-engineers due to their rich set of unique properties, valuable for many high-tech industrial and bio-medical applications. References [20–26] are devoted to the theoretical study of the behavior and properties of such systems, which are of interest both for fundamental studies of nanodisperse systems and for their applications.

In Ref. [20], results of theoretical modeling of dynamic remagnetization of a dimer, consisting of two single-domain ferromagnetic particles immobilized in a non-magnetic medium, are presented. The results show that the formation of the dimers leads to an increase in the system magnetization and to significant growth of the characteristic time of its remagnetization.

Mathematically, a regular model of dynamic susceptibility and magnetoviscous effect in non-dilute polydisperse ferrofluids with magnetically interacting particles is proposed in Ref. [21]. Analysis shows that the dynamic properties of polydisperse systems can differ significantly from those of the model monodisperse ones consisting of the particles, with size equal to the average particle size in the real ferrofluid. Reference [22] deals with a theoretical study of spinodal decomposition and magneto-diffusion transport in thermodynamically unstable systems of nanodisperse ferromagnetic particles. Effects of external magnetic field and the long-ranged interparticle correlations as well as the kinetics of this transformation are analyzed. The appearance of dense structures, aligned along the applied field, is demonstrated.

Magnetic hyperthermia is one of the effective methods of cancer disease therapy. Its key idea is the injection of magnetic nanoparticles into the tumor area and heating of the particles and, therefore, the tumor cells, by an alternating magnetic field. Experiments reveal that inside the cells the embedded particles can form various dense clusters. Reference [23] deals with a theoretical study and modeling of heat production by clustered ferromagnetic nanoparticles.

Reference [24] develops a theoretical background for the intensification of drag transport in a thrombosed blood vessel with the help of injected magnetic nanoparticles and an alternating magnetic field. In addition, the impact of different magnetic materials added to silver-magnetite nanoparticles on the structural, magnetic, and antimicrobial properties is described in Ref. [25].

Finally, Ref. [26] comprehensively summarizes the mechanisms and models of magnetic loss of single-domain magnetic particles in an external magnetic field, provides a convenient reference for researchers to explore the properties of single-domain magnetic particles, and promotes their application and development in the field of biomedicine.

3 Conclusions

The present issue covers multiple disciplines, ranging from the non-equilibrium statistical physics of microscopic effects to phenomenological non-equilibrium thermodynamics, condensed matter physics, and biomedical applications. Special attention is paid to developing the scientific background of biomedical applications.

This issue has a great impact on the research in the field of phase transitions and rheological, transport, synergetic, and other non-equilibrium phenomena in multicomponent disordered and biological systems. New results on these phenomena in disordered matter and materials define a fundamental basis for rapidly developing research in rheological phenomena in field-sensitive fluids and composites, magnetic hyperthermia in biological cells and intracellular tissues, the intracellular cargo transport, non-equilibrium phase, and structural transitions in composite and multi-component matters, and glassy states and transformations, being therefore of broad public interest.

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