

9th World Congress on

MATERIALS SCIENCE AND ENGINEERING

June 12-14, 2017 Rome, Italy

Quasi particle approach to study the kinetics of self-assembly in complex materials

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Statement of the Problem: A self-organization is a universal phenomenon in nature and, in particular, is highly important in materials systems. Our goal was to develop a new theory that provides a computationally effective approach to this problem.

Methodology & Theoretical Orientation: The proposed theory rests on two novel conceptual premises: (1) the introduction of interacting pseudo particles that we call fratons that described two configurational states of each point of continuum space. The fratons are considered as a non-ideal gas whose "condensation" describes a diffusional self- assembling of atomic system, and (b) a concept of a structural cluster function describing the directions, length and strength of interatomic bonds. The latter allows us to formulate a new and simple model Hamiltonian. This Hamiltonian model provides the formation of a predetermined atomic structure and has a sufficient flexibility to describe the desired mechanic and thermodynamic properties of this structure.

Findings: The modeling based on the proposed theory is at atomic resolution, and addresses the time scale commensurate with a typical diffusion time, which may range from a fraction of a second to years. To demonstrate a potentiality and versatility of our approach, we tested its application to a self-assembling of disordered systems to three groups of systems of increasing topological complexity, viz., single component crystals (fcc, hcp and diamond structures), two component crystals (zinc-blend structure), self-assembly of the randomly distributed monomers into single-strand and double-stranded helices and grain boundaries structure. The spontaneous self-organization of fratons into the diamond structure was also observed.

Conclusion & Significance: The developed approach opens a way to answer numerous outstanding questions concerning the atomistic mechanisms of the formation of defects (dislocations, grain boundaries, etc.), nucleation in solid-solid transformations, folding and crystallization of polymers, and their responses to external stimuli.

Biography

H Zapolsky is a Professor of Theoretical Physics at Rouen University, her main research interest lies in theoretical understanding of the emergence of patterns formation and kinetics of phase transformation in different type of materials. Applying different mathematical and computational approaches to diverse problems in materials science she developed an original multiscale tool to study phase transformations in materials. Recently, she proposed a novel statistical-mechanical approach to model a spontaneous self-assembling of randomly distributed atoms into pre-determined atomic structures of almost any complexity.

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