Quasiparticle approach to study the kinetics of self-assembly in complex material

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Abstract

Statement of the Problem: A self-organisation is an 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: (a) the introduction of interacting pseudoparticles 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 model Hamiltonian 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 helixes and grain boundaries structure. The spontaneous self-organisation of fratons into the diamond structure is shown in Figure 1.

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 crystallisation of polymers, and their responses to external stimuli.

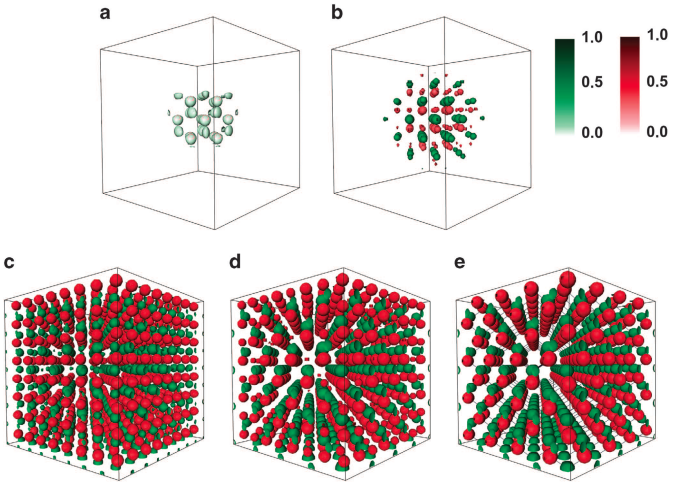


Figure1. Example of a self-assembly of fratons into zinc-blende structure at reduced times t* of (a) t*= 0, (b) t*=160000, (c) t*=190000,(d) t*=280 000 and (e) t*=3000000..

Recent Publications (minimum 5)

1. J. Boisse, H. Zapolsky, A.G. Khachaturyan (2011), «Atomic-scale modeling of nanostructure formation in FeGa alloys with giant magnetostriction: Cascade ordering and decomposition » Acta Materilia ,**59**:2656-2668.
2. O. Kapikranyan, H. Zapolsky, C. Domain, R. Patte, C. Pareige, B. Radiguet, P. Pareige (2014) « Atomic density function modeling of atomic structure of grain boundaries, Phys. Rev. B., **89**: 014111.
3. M. Certain, H. Zapolsky, A.G. Khachaturyan (2011) « Atomic density function simulations of crystal growth kinetics of FCC crystal and FCC-BCC transition », Solid State Phenomena, **172 – 174**:1234-1239.
4. H. Zapolsky (2015) "Kinetics of pattern formation: mesoscopic and atomistic modelling" ORDER, DISORDER AND CRITICALITY, Advanced Problems of Phase Transition Theory, Volume IV, ,pp 153-193, Ed. Y. Holovach, World Scientific Publishing Co.
5. O. Kapikranian, H. Zapolsky, R. Patte, C. Pareige, B. Radiguet, and P. Pareige (2015) "Point defect absorption by grain boundaries in alpha iron by atomic density function modelling" Phys.Rev.B **92**: 224106.
6. M. Lavrskyi, H. Zapolsky, A.G. Khachaturyan (2016) « Quasiparticle Approach to Diffusional Atomic Scale Self-Assembly of Complex Structures: from Disorder to Complex Crystals and Double Helix Polymers », Nature Parther Journal Computational Materials, 14 January.



Biography (150 word limit)

Helena 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 a pre-determined atomic structures of almost any complexity. 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. This method has been applied to describe the segregation at grain boundaries, self-assembly of the randomly distributed monomers into single-strand and double-stranded helixes and phase transformations in binary and ternary alloys.

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Notes/Comments: