Final Report of the project KKP-126749 entitled Modeling crystal morphology at various length scales: From atomic scale to biological systems

January 29, 2024

This "Frontline - Research Excellence Programme" project was awarded to our renowed colleague, Prof. László Gránásy. He led the work with great profession and enthusiasm but unfortunately he could not put the finishing touches to it himself, because he passed away two months before the termination of the project. The following report was written based on the contributions from the other senior researchers, summarizing the work in chapters corresponding to the main subjects of our studies. The details are available in the respective publications, each cited with the number it appears in the publication list prepared separately, as compulsory part of the online submission of this Final Report. For the convenience of the reviewer, this list is attached to the end of this document.

Nucleation

We reviewed how the conventional phase-field models, that rely on coarse grained order parameters, and the phase-field-crystal models, that work on the molecular scale while employing time averaged particle densities, contributed to the understanding of various aspects of crystal nucleation. The examples, which were selected mostly from our simulations, include homogeneous and heterogeneous nucleation, precursor assisted nucleation, nucleation in eutectic and in phase separating systems, phase selection via competing nucleation processes, growth front nucleation (a process, in which grains of new orientations form at the solidification front) yielding crystal sheaves and spherulites, and transition between the growth controlled cellular and the nucleation dominated equiaxial solidification morphologies [Ref. 7].

To help in comparing the accuracy and efficiency of the different simulation codes used in the phase-field community, we proposed several standardized nucleation scenarios as benchmark problems: homogeneous nucleation with a single seed or multiple seeds, and athermal heterogeneous nucleation where the behavior of a solid seed near the free growth limit is investigated [Ref. 23].

We investigated two-step nucleation and post-nucleation growth in the framework of phase-field crystal (PFC) models supplemented with diffusive dynamics (DPFC, corresponding to colloid suspensions) or linearized hydrodynamics (HPFC, corresponding to simple liquids). The structure of the appearing solid was analyzed via the $\overline{q}_6$ average bond order parameter, distinguishing between amorphous, medium range crystallike order (MRCO), and crystalline local orders. We have observed that in both models first an amorphous structure appears, followed by the formation of MRCO, which precede the formation of the stable bcc structure (see Fig. 1). The post-nucleation and planar interface growth rates predicted by the different models

were also compared. We found, that nucleation and the post nucleation behavior appear to be less sensitive to the mechanism of density relaxation than the kinetics of crystal growth. This is so, despite the fact that in the present studies nucleation took place via intermediate states preferred kinetically relative to direct bcc nucleation [Ref. 16].

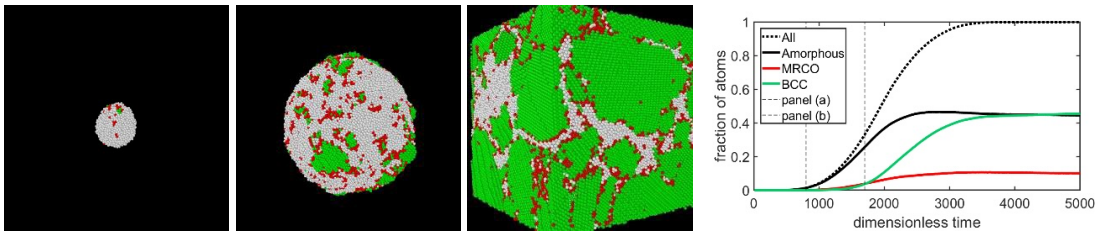

Figure 1: Nucleation and growth in the HPFC model. The left three snapshots show the growth of a single solid particle, while the graph on the right shows the time evolution of the volume fractions of different structures in the whole simulation volume. Colors on the left correspond to the colors on the right [Ref. 16].

Within the framework of the HPFC model, we further investigated the early stage of cluster formation. In addition to the amorphous structure seen before, we identified a layered 2D quasicrystal-like structure that is periodic in the third dimension, and we found that the stable bcc phase nucleates on these structures in a heterogeneous manner. Using this model, we also searched for a possible analogue of satellite crystal formation in the vicinity of the growth front, a phenomenon discovered in molecular dynamics simulations. We found that interference of density waves ahead of the growth front of uneven shape may assist crystal nucleation, even if bulk homogeneous nucleation is not yet active. We also investigated heterogeneous nucleation on a circular substrate in the presence of fluid flow. Under appropriate conditions, fluid flow may tear off heterogeneously nucleated crystal particles from the surface of a curved substrate, as seen in colloidal systems [Ref. 24].

The properties of the amorphous solid has been further investigated in the framework of the phase-field crystal model. With extensive numerical simulations, we determined the distribution of free energy density values in amorphous systems of varying size. We found that in the thermodynamic limit, the free energy density of the amorphous tends toward a value that has a slight dependence on the initial state from which it was formed. The liquid to amorphous transition is found to be first order, with an associated finite free energy barrier when the liquid is metastable. This is also demonstrated by inducing nucleation events by adding noise to the initial density distribution. Depending on the strength of the noise, we observed a variety of nucleation pathways, in agreement with previous results for the PFC model, which showed that amorphous precursor mediated multi-step crystal nucleation can occur in colloidal systems [Ref. 28].

Structure of single particle biomolecules

Determining the structure of biological molecules is often hindered by the fact that they cannot be crystallized. In these cases, the required structural information can be obtained by recording the diffraction pattern of a large number of identical particles injected into the X-ray free-electron laser (XFEL) beam in random orientations. The crucial step of the data processing is finding the orientations of the recorded diffraction patterns in reciprocal space and reconstructing the 3D intensity distribution. We compared two orientation methods: the expansion maximization compression (EMC) algorithm and the correlation maximization (CM) algorithm in terms of efficiency, reliability and accuracy using simulated diffraction patterns

of biological molecules [Ref. 20].

Phase transitions in systems with competing short- and long-range interactions.

Motivated by experiments on cold atoms in an optical cavity low dimensional systems incorporating both nearest neighbor and global range interactions are studied. For hard-core bosons formation of a dynamically generated supersolid state was explored by exact calculations in one-dimensional systems [Ref. 1]. For a related spin-1/2 XX model we have also determined the quantum relaxation properties of the system after sudden quenches and properties of non-equilibrium phase transitions have been exactly calculated [Ref. 2].

Low-energy properties of disordered quantum systems

Disorder is an inevitable feature of real materials. Its presence can drastically change the low-energy, low-temperature properties of these systems. Using different numerical techniques (DMRG, combinatorial optimization and strong disorder RG (SDRG) methods) we explored the phase diagram of quantum Ising chain with uniformly distributed random antiferromagnetic couplings and uniformly distributed random transverse fields in the presence of a homogeneous longitudinal field [Ref. 12]. We calculated the distribution of the excitation energy of the random transverse Ising chain in the disordered Griffiths phase by the SDRG method and – for shorter chains – by free-fermion techniques and the results are compared with the predictions of extreme statistics [Ref. 17]. We studied the geometrical properties of rare regions in the transverse Ising model with dilution or with random couplings and transverse fields and studied their relation with the low-temperature properties of the system [Ref. 25]. Motivated by the compound $LiHo_xY_{1-x}F_4$, we considered an Ising chain with random couplings in the presence of simultaneous random transverse and longitudinal fields, and studied its low-energy properties at zero temperature by the SDRG approach [Ref. 33]. New developments in the application of the SDRG method – including random quantum magnets, classical disordered systems and stochastic models with quenched disorder – are summarized in our review paper [Ref. 3]. We have written a popular science review on the present knowledge on glass formation and the structure of the free energy surface of glasses [Ref. 27].

Entanglement entropy and related topics

Entanglement is a key ingredient of the characterization of a quantum system. In a quantum system a finite, connected (hypercubic) domain of linear extent L, the points of which belong to the subsystem with probability p was considered in one- and two dimensions and the leading contribution to the average entanglement entropy is calculated [Ref. 10]. We used entanglement witnesses to detect entanglement in the XY-chain in thermal equilibrium and determine the temperature bound, below which the state is detected as entangled. We also studied the post-quench states in the thermodynamic limit after changing the parameters of the Hamiltonian suddenly [Ref. 30]. We investigated mixed-order transition in the antiferromagnetic quantum Ising chain in the presence of a longitudinal field, a scenario that was recently experimentally realized by ultracold atoms in an optical lattice. We have theoretically checked the properties of the phase transition of this model [Ref. 21].

Pattern formation in eutectic and biological systems

The solidification of eutectic systems provide some well known examples for self-organised pattern formation, including the lamellar and rod two-phase structures. In some cases, e.g., during the layer-wise building up of components by additive manufacturing, the melting of these structures can also play an important role in determining the final microstructure. We made analytic and numerical studies to explore the details of the melting process takes place in eutectic materials [Ref. 29].

Statistical physical modeling was used to describe pattern formation in light emitting bacterium colonies, which show transitions akin to phase transitions [Ref. 13]. Performing Monte Carlo simulations, we studied the properties of the transition in a correlated percolation model [Ref. 18]. Using combinatorial optimization techniques, we studied the critical properties of a related system, the two- and three-dimensional Ising models with uniformly distributed random antiferromagnetic couplings in the presence of a homogeneous longitudinal field, h, at zero temperature [Ref. 26].

Complex morphologies, biomineralization

The formation of 3D mineral–organic functional architectures by living organisms is a tremendously active research field spanning many scientific disciplines. As a result of millions of years of evolution, mollusks, as well as many other animals, gained the ability to shape mineral crystals into unconventional morphologies very efficiently. The role of the organisms in the formation of these structures is not to conduct the crystallization process directly, rather to provide the required conditions, such as the protected region, the right composition and pH, for thermodynamically driven self-assembly. This opens the hope to use traditional materials science tools, such as phase-field modeling, to describe the process.

Taking the freshwater mussel *Unio pictorum* as example, the growth of the shell starts with the formation of a granular layer, transforming to a prismatic and later to a nacreous layer consisting of aragonite ($CaCO_3$) and chitin. This composite structure provides excellent mechanical properties for the protection of the animal. To describe this growth form, we performed 2D simulations of structural evolution during the solidification of the shell within the framework of a phase-field model that was previously successfully employed to describe complex polycrystalline morphologies. We demonstrated (see Fig. 2) that the observed layered structure can be reproduced in a model binary system, by providing an outer surface for nucleation to initiate the inwards growth of the crystalline phase, and by assuming a smooth change in the liquid composition, i.e, in the driving force. Structural development of the shell in thickness was shown to be the result of a transition from a fast to a slow directional solidification mode, accompanied by an increased morphological regularity [Refs. 5, 19].

As a next step, we improved our model by using a moving boundary on the liquid side of the 2D domain. In molluscs, crystallization proceeds in a thin, liquid filled cavity, the extrapallial space between the biomineralizing front and mantle tissue covering it. We modelled this scenario by moving the boundary of the domain at a rate which provided a constant thickness for the liquid layer ahead of the crystallizing front. The composition of the liquid is then adjusted via varying the boundary condition along this moving boundary. By assuming that the animal controls the $CaCO_3$ supersaturation at the mantle, decreasing it exponentially with time, morphologies resembling the layered structures of shells from three major molluscan classes, the bivalve *Unio pictorum*, the cepalophod *Nautilus pompilius*, and the gastropod *Haliotis asinina* could be reproduced [Refs. 9, 19].

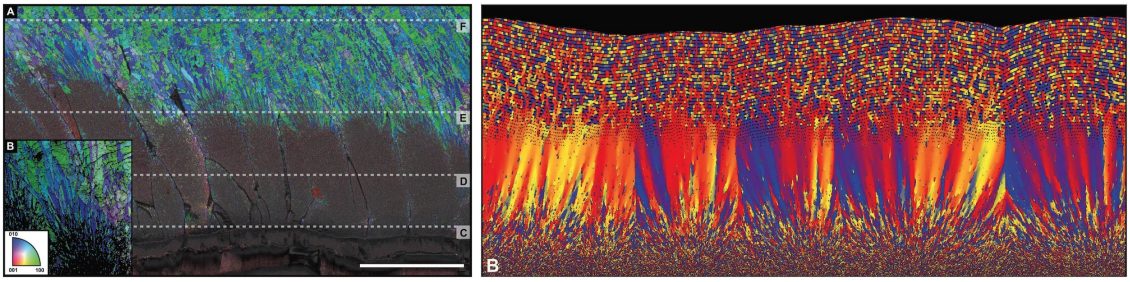

Figure 2: The layered structure of the shell of *Unio pictorum*. EBSD map (left) vs. our phase-field simulations [Ref. 5].

Then we focused on the formation of the nacre. Now it was assumed that the organic sheets that separate the mineral tablets in the final structure are already present when crystallization of aragonite takes place. The crystallization front may traverse through these organic sheets via holes in them, and depending on the position where these holes are formed, the final morphology of the nacre can be very different. In the columnar nacre (found in gastropods and cephalopods) these holes are aligned along the column centers, while in sheet nacre (seen in bivalves) they are at seemingly random positions. With our phase field model, treating the organic layers with the holes as the boundary of the simulation domain, we could successfully reproduce these two different kinds of nacre structures (see Fig. 3). In addition, we showed how the model parameters, such as anisotropy, wetting properties, etc. can further influence the final structure [Ref. 31].

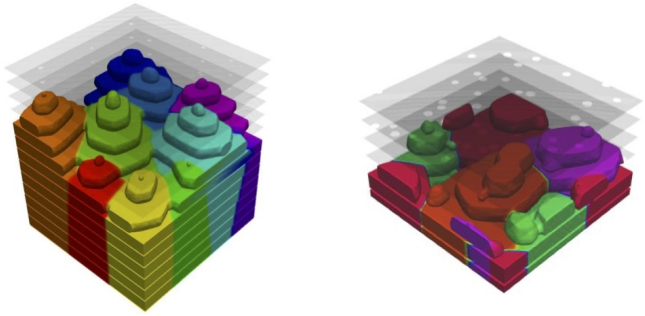

Figure 3: Phase-field modeling of the formation of columnar (left) vs. sheet nacre (right). In both cases, crystallization of aragonite tablets (shown in colors depending on their crystallographic orientation) happens in thin layers between parallel organic sheets (gray). Unpublished images similar to those in Ref. 31.

Another area of biomineralization where we successfully used our materials science expertise was in help explaining the microstructure formation of coral skeletons. Stony corals are morphologically diverse at the centimeter scale, but reveal morphological similarities on the microscopic scale. They are well known to form their skeletons from aragonite spherulites, displaying needle-like aragonite crystal fibers radiating from centers of calcification. We proposed a new growth mechanism for these spherulitic structures, instead of the previously assumed non-crystallographic branching. In this, at the growth front, small grains, "sprinkles" are formed by random orientation, which grow further by competing for space and also coarsen in the bulk crystal. This mechanism is strongly supported by our phase-field simulations (see Fig. 4), and explain the microstructural variations across species via changes in the thermodynamic parameters. Interdisciplinary research combining experimental and theoretical techniques can be a particularly powerful approach for elucidating the fundamental mechanisms of crystal nucleation and growth [Refs. 15, 19].

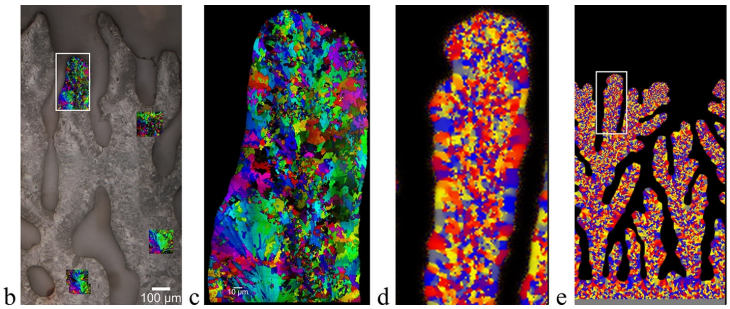

Figure 4: Comparison of the cross sectional microstructure of the skeleton of coral species *Balanophyllia europea* (b,c) to our phase-field simulations (d,e). Different colors correspond to different crystallographic orientation [Ref. 15].

Pattern formation and anisotropy in convecting medium

Sponge-like structures commonly occur in biological and artificial self-assembled systems, which are characterized by two bi-continuous phases. A possible route to create such inter-percolating structures is allowing phase separation in a multi-component systems. It is generally acknowledged, that varying the composition (i.e. the fraction of the phases) leads to either dispersed or bi-continuous phases at asymmetric and close to symmetric phase fractions, respectively. However, in most investigations, the viscosity of the phases are kept constant, irrespective of the composition. We have shown that applying concentration dependent viscosity has significant effect on the patterning regimes of the phase-separation, causing asymmetric regimes in the dispersed/bi-continuous phase diagram [Refs. 4, 6]. We could also used this technique to study phase separation in systems with technological interest [Ref. 22].

According to recent studies, calcium carbonate in biological systems may not directly crystallize directly from Ca^{2+} and CO_3^{2-} ions, but forming amorphous $CaCO_3$ grains first. The transport and ordering of these grains through a fluid medium may influence the crystallization process and therefore the biomineralized structure. To be able to simulate the growth of a solid particle that moves with the flow in the liquid, we developed a model which combines the phase-field and the lattice Boltzmann methods [Refs. 8, 32]. In the framework of fluid-structure interaction (FSI) direct simulations we have examined the scenario of orientational ordering of anisotropic grains. In a simple case when elongated elliptic particles interacting with sheared medium; it was shown that orientational order is present in the system. Two distinct regimes are identified: in the case of a highly viscous medium the particles rotating similar to Jefferey orbits, while below a viscosity threshold the particles have a small steady angle to the direction of shearing. The latter regime displays very pronounced ordering in the elongated particle suspension [Ref. 11].

Scientometric data

We published 32 papers in international, peer reviewed journals and 1 article in a Hungarian popular science journal. The sum of the impact factor of these publications is 191 and, at the time of submitting this report, they have 366 independent citations registered in the Hungarian Science Bibliography (MTMT).

PROJEKT ZÁRÓ BESZÁMOLÓ
közlemények

NKFI-azonosító: 126749	Típus: KKP
Szakmai jelentés:	

Vezető kutató: Pusztai Tamás	Kutatóhely: SZFI - Kísérleti Szilárdtest-fizikai Osztály (HUN-REN Wigner Fizikai Kutatóközpont)

Zsűri: KKP	Kezdet: 2018. 01. 01	Teljes kutatási időszak: 2018-01-01 - 2023-12-31	Főkönyviszám: 71115	Nyomtatás: 2024. 01. 26.

NEM VÉGLEGESÍTETT VÁLTOZAT!!!

Sorszám	Közleményjegyzék	Dokumentum típusa	Impakt faktor	NKFI támogatás feltüntetve?	Támogató szervezetek
1.	B. Blass, H. Rieger, G. Roósz, F. Iglói: ***Quantum relaxation and metastability of lattice bosons with cavity-induced long-range interactions***, Phys. Rev. Lett. 121, art. no. 095301 (pp. 1-6), 2018	folyóiratcikk	8.839	igen	Saarland University
2.	F. Iglói, B. Blass, G. Roósz, H. Rieger: ***Quantum XX-model with competing short- and long-range interactions: Phases and phase transitions in and out of equilibrium***, Phys. Rev. B 98, art. no. 184415 (pp. 1-15), 2018	folyóiratcikk	3.813	igen	Saarland University
3.	F. Iglói, C. Monthus: ***Strong disorder RG approach - a short review of recent developments***, Eur. Phys. J. B 91, art. no. 290 (pp. 1-25), 2018	folyóiratcikk	1.536	igen	
4.	H. Henry, G. Tegze: ***Self-similarity and coarsening rate of a convecting bicontinuous phase separating mixture: Effect of the viscosity contrast***, Phys. Rev. Fluids 3, 074306 (pp. 1-9), 2018	folyóiratcikk	2.021	igen	École Polytechnique, Palaiseau, Grand Équipement National de Calcul Intensif
5.	V. Schoeppler, L. Gránásy, E. Reich, N. Poulsen, R. de Kloe, P. Cook, A. Rack, T. Pusztai, I. Zlotnikov: ***Biomineralization as a paradigm of directional solidification: A physical model for molluscan shell ultrastructural morphogenesis***, Adv. Mater. 45, art. no. 1803855 (pp. 1-8), 2018	folyóiratcikk	25.809	igen	Technische Universität Dresden, European Synchrotron Radiation Facility, Bundesministerium für Bildung und Forschung
6.	H. Henry, G. Tegze: ***Kinetics of coarsening have dramatic effects on the microstructure: Self-similarity breakdown induced by viscosity contrast***, Phys. Rev. E 100, art. no. 013116 (pp. 1-10), 2019	folyóiratcikk	2.353	igen	CNRS, IDRIS
7.	L. Gránásy, G.I. Tóth, J.A. Warren, F. Podmaniczky, G. Tegze, L. Rátkai, T. Pusztai: ***Phase-field modeling of crystal nucleation in undercooled liquids – A review.***, Prog. Mater. Sci. 106, art. no. 100569 (pp. 1-51), 2019	folyóiratcikk	31.560	igen	
8.	L. Rátkai, T. Pusztai, L. Gránásy: ***Phase-field lattice Boltzmann model for dendrites growing and moving in melt flow.***, Nature partner journal Comput. Mater. 5, art. no. 113 (pp. 1-10), 2019	folyóiratcikk	9.341	igen	European Space Agency
9.	V. Schoeppler, R. Lemanis, E. Reich, T. Pusztai, L. Gránásy, I. Zlotnikov: ***Crystal growth kinetics as an architectural constraint on the evolution of molluscan shells***, PNAS (Proc. Nat. Acad. Sci. U.S.A.) 114, (41) art. no. 2019-07229RR (pp. 1-10), 2019	folyóiratcikk	9.412	igen	Bundesministerium für Bildung und Forschung, Deutsche Forschungsgemeinschaft, Technische Universität Dresden
10.	G. Roósz, I. A. Kovács and F. Iglói: ***Entanglement entropy of random partitioning***, Eur. Phys. J. B 93, art. no. 8 (pp. 1-8), 2020	folyóiratcikk	1.347	igen	Deutsche Forschungsgemeinschaft, John Templeton Foundation
11.	G. Tegze, F. Podmaniczky, E. Somfai, T. Börzsönyi, L. Gránásy: ***Alignment of rigid elongated particles in sheared non-Brownian suspensions.***, Soft Matter 16, 8925-8932, 2020	folyóiratcikk	3.399	igen	
12.	P. Lajkó, J.-Ch. Anglés d'Auriac, H. Rieger, F. Iglói: ***Reentrant random quantum Ising antiferromagnet***, Phyical Review B 101, art. no. 024203, (pp. 1-9), 2020	folyóiratcikk	3.575	igen	Institut Néel, Grenoble, Saarland University
13.	P. Maróti, I.A. Kovács, M. Kiss, J.L. Smart, F. Iglói: ***Correlated clusters of closed reaction centers during induction of intact cells of photosynthetic bacteria***, Sci. Reports 10, art. no. 14012, (pp. 1-16), 2020	folyóiratcikk	3.998	igen	EFOP, University of Szeged Open Access Fund, Hungarian Academy of Sciences, John Templeton Foundation
14.	R. Zanella, G. Tegze, R. Le Tellier, H. Henry: ***Two- and three-dimensional simulations of Rayleigh–Taylor instabilities using a coupled Cahn–Hilliard/Navier–Stokes model***, Phys. Fluids 32, art. no. 124115, (pp. 1-13), 2020	folyóiratcikk	3.514	igen	Commissariat à l'énergie atomique et aux énergies alternatives, Electricité de France
15.	C.-Y. Sun, L. Gránásy, C.A. Stifler, T. Zaquin, R.V. Chopdekar, N. Tamura, J.C. Weaver, J. Zhang, S. Goffredo, G. Falini, M.A. Marcus, T. Pusztai, V. Schoeppler, T. Mass, P.U.P.A. Gilbert: ***Crystal nucleation and growth of spherulites as revealed by coral skeletons and phase-field simulations***, Acta Biomater. 120, 277-292, 2021	folyóiratcikk	8.947	igen	US DOE, NSF, ERC Grants, US-Israel Binational Science Fund
16.	F. Podmaniczky, L. Gránásy: ***Nucleation and post-nucleation growth in diffusion-controlled and hydrodynamic theory of solidification***, Crystals 11, art. no. 437 (pp. 1-14), 2021	folyóiratcikk	2.670	igen	
17.	I.A. Kovács, T. Pető, F. Iglói: ***Extreme statistics of the excitations in the random transverse Ising chain***, Phys. Rev. Res. 3, art. no. 033140 (pp. 1-10), 2021	folyóiratcikk	3.900	igen	European Social Fund, Hungarian Government
18.	J.-C. A. d'Auriac, F. Iglói: ***Statistics of percolating clusters in a model of photosynthetic bacteria***, Phys. Rev. E 103, art. no. 052103 (pp. 1-6), 2021	folyóiratcikk	2.529	igen	
19.	L. Gránásy, L. Rátkai, G. I. Tóth, P.U.P.A. Gilbert, I. Zlotnikov, T. Pusztai: ***Phase-field modeling of biomineralization in mollusks and corals: Microstructure vs. formation mechanism***, J. Am. Chem. Soc. Au 1, 1014-1033, 2021	folyóiratcikk	8.000	igen	Hungarian Academy of Sciences (MTA), US. Department of Energy, US. NSF Biomaterials, Bundesministerium für Bildung und Forschung
20.	M. Tegze, G. Bortel: ***Comparison of EMC and CM methods for orienting diffraction images in single-particle imaging experiments***, IUCrJ 8, 980-991, 2021	folyóiratcikk	4.769	igen	Hungarian Academy of Sciences
21.	P. Lajkó, F. Iglói: ***Mixed-order transition in the antiferromagnetic quantum Ising chain in a field***, Phys. Rev. B 103, art. no. 174404 (pp. 1-8), 2021	folyóiratcikk	4.036	igen	
22.	R. Zanella, R. Le Tellier, M. Plapp, G. Tegze, H. Henry: ***Three-dimensional numerical simulation of droplet formation by Rayleigh–Taylor instability in multiphase corium***, Nuclear Eng. Des. 379, art. no. 111177 (pp.1 - 9), 2021	folyóiratcikk	2.040	igen	Ecole Polytechnique, CNRS PICS program
23.	W. Wu, D. Montiel, J.E. Guyer, P.W. Voorhees, J.A. Warren, D. Wheeler, L. Gránásy, T. Pusztai, O.G. Heinonen: ***Phase field benchmark problems for nucleation***, Comput. Mater. Sci. 193, art. no. 110371 (pp. 1-11), 2021	folyóiratcikk	3.300	igen	U.S. Department of Commerce, U.S. Department of Energy, Laboratory Computing Resource Center at Argonne National Laboratory
24.	F. Podmaniczky, L. Gránásy: ***Molecular scale hydrodynamic theory of crystal nucleation and polycrystalline growth***, J. Cryst. Growth 579, art. no. 126854 (pp. 1-8), 2022	folyóiratcikk	1.814	igen	European Space Agency, Hungarian Academy of Sciences
25.	I. Kovács, F. Iglói: ***Geometry of rare regions behind Griffith singularities in random quantum magnets***, Scientific Reports - Nature 12, art. no. 1074 (pp. 1-10), 2022	folyóiratcikk	4.379	igen	
26.	J.-C.A. d'Auriac, F. Iglói: ***Random-bond antiferromagnetic Ising model in a field***, Phys. Rev. E 106, art. no. 034117 (pp. 1-6), 2022	folyóiratcikk	2.707	igen	
27.	K, Binder, F. Iglói: ***Az üvegátalakulás: Hogyan jelennek meg hegyek és völgyek a szabadenergia felszínén***, Fizikai Szemle 72, pp. 161-166, 2022	folyóiratcikk	-	igen	
28.	S. Abdalla, A. Archer, L. Gránásy, G.I. Tóth: ***Thermodynamics, formation dynamics and structural correlations in the bulk amorphous phase of the phase-field crystal model***, J. Chem. Phys. 157, art. no. 164502 (pp. 1-13), 2022	folyóiratcikk	4.304	igen	EPSRC (U.K.)
29.	T. Pusztai, L. Rátkai, L. Horváth, L. Gránásy: ***Phase-field modelling of directional melting of lamellar and rod eutectic structures.***, Acta Mater. 55, art. no. 117678 (pp. 1-10), 2022	folyóiratcikk	8.203	igen	European Space Agency
30.	F. Iglói and G. Tóth: ***Entanglement witnesses in the X Y chain: Thermal equilibrium and postquench nonequilibrium states***, Phys. Rev. Research 5, 013158, 2023	folyóiratcikk	4.200	igen	EU, Spanish MCIU, Spanish Ministry of Science, Basque Government
31.	Gránásy L., Rátkai L., Zlotnikov I., Pusztai T.: ***Physical Phenomena Governing Mineral Morphogenesis in Molluscan Nacre***, SMALL 2304183, 2023	folyóiratcikk	13.300	igen	
32.	L. Rátkai, L. Gránásy, T. Pusztai: ***Phase-field lattice Boltzmann model of growth and buoyancy driven motion of dendritic particles: the effect of Coriolis force***, IOP Conference Series: Materials Science and Engineering, 2023	folyóiratcikk	0.500	igen	European Space Agency
33.	T. Pető, F. Iglói, I. A. Kovács: ***Random Ising chain in transverse and longitudinal fields: Strong disorder RG study***, Condensed Matter Physics, vol. 26, No. 1, 13102, 2023	folyóiratcikk	0.600	igen	