Исследование выполнено за счет гранта Российского фонда фундаментальных исследований (проект № 18-32-00550). Также данная работа поддержана Актом 211 Правительства Российской Федерации, контракт № 02.A03.21.0006.

1. Vokhmintsev A.S., Weinstein I.A., Minin M.G., Shalyakin S.A., Radiation Measurements, 124, 35 (2019)
2. Vokhmintsev A.S., Weinstein I.A., Zamyatin D.A., Journal of Luminescence, 208, 363 (2019)
3. Spiridonov D.M., Henaish A.M.A., Shalyakin S.A., Vokhmintsev A.S., Weinstein I.A., Journal of Physics: Conference Series, 1115, 5, 052025 (2018)

STOCHASTIC MODIFICATION OF THE MPFC MODEL

Starodumov I.[1], Alexandrov D.[1], Galenko P.[1, 2], Nizovtseva I.[1, 2], Ivanov A.[1]

[1)] Laboratory of Multi-Scale Mathematical Modeling, Ural Federal University, Ekaterinburg, Russia
[2)] Friedrich-Schiller-Universitat Jena, Physikalisch-Astronomische Fakultat, Jena, Germany
E-mail: ilya.starodumov@urfu.ru

The mathematical modeling of crystal structures and their dynamics during the structural transitions can be performed by the method of phase field crystal in the hyperbolic formulation (MPFC method). We propose the stochastic extension of MPFC-model to find the effect of atomic fluctuations.

The mathematical modeling of crystal structures and their dynamics during the structural transitions can be performed by the method of phase field crystal in the hyperbolic formulation (MPFC method). The model can be considered from the Swift-Hohenberg equation and the Density Functional Theory. This method is suitable for a continual modeling of the atomic density field at diffusion time intervals. The unstable behavior of the solution near local energy minima is discussed.

The authors propose the hypothesis of the formation of metastable structures during the relaxation of domain to the stable state. Due to the presence of the set of different possible structures on the system's transformation path, the pattern of the atomic density field could remain still when the system is in the vicinity of local free energy minima [1,2].

To perform reliable simulations, one should take into account the factors leading to the appearance of instability. Special additional term for describe atomic vibrations in the field of atomic density should allow the system to come out of metastable states and increase the rate of formation of equilibrium and stable states consistent with diagrams of structures. The approach of introducing the noise as a fluctuation effect developed for the WCT and mean-field theories may be utilized in the PFC model. The narrow approach of introducing the noise-terms in the stochastic hyperbolic phase-field models [3] could be used as a base for the physically-consisted fluctuations.

We propose the simple stochastic modification of hyperbolic PFC-model to find the effect of fluctuations on the dynamics of atomic density field. Results of simulations in presence and in lack of noise indicate that the moderate noise of the atomic density field amplitude could provide the quick relaxation.

Authors acknowledge the support by the Russian Science Foundation under the project no. 19-71-10044.

1. I. Starodumov, P. Galenko, N. Kropotin, D. V. Alexandrov, “Influence of initial seed distribution on the pattern formation of the phase field crystals” AIP Conference Proceedings, 1906, 200006 (2017).
2. I. Starodumov, D. Alexandrov, and E. Pavlyuk, “On the stability of high-performance crystal growth simulations by the MPFC method”, AIP Conference Proceedings, 1997, 020065 (2018).
3. D. Kharchenko, I. Lysenko, P. Galenko, “Fluctuation effects on pattern selection in the hyperbolic model of phase decomposition”, Stochastic Differential Equations, (2011).