

# KINETICS OF NANOPORE GENERATION

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**Abstract:** The nucleation of nanopores in materials is studied as the initial stage of a phase transition that causes microstructure amorphization of a solid surface thin layer under the influence of pulsed ion fluxes of inert gases. Computer experiments are based on solutions of the kinetic theory equations of Fokker–Planck–Kolmogorov and stochastic Ito equations with nonlinear functional coefficients. The porosity structures in the samples depend on the types of the material crystal lattices and the layer sizes, the sample temperature, the ion energy values, and the intensity of their flux. The nonequilibrium of the fluctuationally unstable processes as well as spatially nonuniform distribution functions of pore sizes indicate a deviation of porosity from monodispersity which may change the assessment of gas permeability in filtration combustion model.

**Keywords:** porosity; vacancy–gas defects; stochastic Ito equations; phase transition nuclei; clustering; stochastic diffusion; kinetic theory; ion implantation; dispersion; pore gas filling

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## Figure Captions

**Figure 1** Isoprojection of the evolution of the distribution function  $(g, t)/f(g, t = 0)$  level surfaces onto the  $\{G0T\}$  plane at the initial stage of phase transition at  $T/T_{\text{melt}} = 0.53$  in the 3C–SiC/Mo layer. The sizes of pore-nuclei clusters are plotted on the abscissa axis, and the time intervals  $[0; T_{\text{finish}}]$  are plotted along the ordinate axis, the time step is  $t_g = 10^{-8}$  s. The porosity varies within a thin 3C–SiC layer, the position of which shifts by 3 nm relative to the “silicon carbide – metal” interface (see Fig. 2)

**Figure 2** Histograms of the void fraction for phase transition in the 3C–SiC/Mo sample at time  $t = 0.02T_{\text{finish}}$  (a) and the void fraction of the layers (b) at time  $t = T_{\text{finish}}$ . Porosity is concentrated in a thin 3C–Si layer located at a distance of 3 nm from the “silicon carbide – metal” boundary

## References

1. Frolov, S. M. 2008. Combustion science and problems of contemporary power engineering. *Russ. J. Gen. Chem.* 79(11):2556–2561. doi: 10.1134/S1070363209110437. EDN: MWWUHB.
2. Zmievszkaya, G. I., A. L. Bondareva, V. D. Levchenko, and T. V. Levchenko. 2007. A kinetic stochastic model of blistering and nanofilm islands deposition: Self-organization problem. *J. Phys. D Appl. Phys.* 40:4842–4849. doi: 10.1088/0022-3727/40/16/013.
3. Bondareva, A. L., G. I. Zmievszkaya, and V. D. Levchenko. 2006. Stochastic model applied to plasma-surface interaction’s simulation. *Eur. Phys. J. D* 38:143–149. doi: 10.1140/epjd/e2006-00044-0.
4. Zmievszkaya, G. I., T. A. Averina, and A. L. Bondareva. 2015. Numerical solution of stochastic differential equations in the sense of Stratonovich in an amorphization crystal lattice model. *Appl. Numer. Math.* 93:15–29. doi: 10.1016/j.apnum.2014.05.006.
5. Zmievszkaya, G. I. 2020. Nonequilibrium kinetics of the initial stage of a phase transition. *Phys. Solid State* 62(1):42–47. doi: 10.1134/S1063783420010394.
6. Leontovich, M. A. 1983. *Vvedenie v termodinamiku. Statisticheskaya fizika* [Introduction to thermodynamics. Statistical physics]. Moscow: Nauka. 416 p.
7. Skorokhod, A. V. 1983. *Stokhasticheskie uravneniya dlya slozhnykh sistem* [Stochastic equations for complex systems]. Moscow: Nauka. 192 p.
8. Arnold, L. 1998. *Random dynamic systems*. Springer monographs in mathematics ser. Springer. 586 p.
9. Sigov, Yu. S. 2001. *Vychislitel’nyy eksperiment: most mezhduduproshlym i budushchim fiziki plazmy. Izbrannyye trudy* [Computational experiment: A bridge between the past and future of plasma physics. Selected works]. Comp. G. I. Zmievszkaya and V. D. Levchenko. Moscow: Fizmatlit. 288 p.
10. Zmievszkaya, G. I. 1996. Chislennyye stokhasticheskiye modeli neravnovesnykh protsessov [Numerical stochastic models of nonequilibrium processes]. *Matematicheskoe modelirovanie* [Mathematical Modeling] 8(11):3–40. Available at: <https://www.mathnet.ru/rus/mm/v8/i11/p3> (accessed February 22, 2026).
11. Artemiev, S. S. 1994. Stability of numerical methods for solving stochastic differential equations. *Siberian Math. J.* 35(6):1070–1074. doi: 10.1007/BF02104707.
12. Zmievszkaya, G. I., and A. L. Bondareva. 2011. Crystalline islands of semiconductor films. *Plasma Physics Reports* 37:87–95. doi: 10.1134/S1063780X10121098.
13. Zmievszkaya, G. I., A. L. Bondareva, V. V. Savchenko, and T. V. Levchenko. 2012. Computer simulation of the origin of porosity. *Numerical analysis of heat and mass transfer in porous media*. Eds. J. M. P. Q. Delgado, A. G. B. Lima,

- and M. Vázquez Silva. Advanced structured materials book ser. Berlin, Heidelberg: Springer. 27:253–274.
14. Zmievskaia, G. I., A. L. Bondareva, and V. V. Savchenko. 2014. Radiation damaging of 3C–SiC lattice: Computer simulation of Brownian motion of non-point defects. *Defect Diffus. Forum* 353:148–152. doi: 10.4028/www.scientific.net/DDF.353.148.
  15. Zmievskaia, G. I., A. L. Bondareva, T. V. Levchenko, and G. Maino. 2015. Computational stochastic model of ions implantation. *AIP Conf. Proc.* 1648:230003. doi: 10.1063/1.4912495.
  16. Zmievskaia, G. I., and A. L. Bondareva. 2016. Kinetics of the formation of pores and a change in the properties of materials in numerical models. *J. Surf. Invest. — X-Ray* 10(4):802–808. doi: 10.1134/S102745101604039X.
  17. Zel'dovich, Ya. B. 1942. K teorii obrazovaniya novoy fazy. Gomogennaya nukleatsiya. Kavitatsiya [On the theory of new phase formation. Cavitation]. *ZhETF* [J. Exp. Theor. Phys.] 12(11–12):525–538.
  18. Lifshitz, E. M., and L. P. Pitaevskii. 1981. *Physical kinetics. Course of theoretical physics*. Transl. J. B. Sykes and R. N. Franklin. Oxford: Pergamon Press. Vol. 10. 452 p.
  19. Golovan, L. A., V. Yu. Timoshenko, and P. K. Kashkarov. 2007. Optical properties of nanocomposites based on porous systems. *Phys. — Usp.* 50(6):595–612.
  20. Andrievsky, R. A. 2012. Osnovy nanostrukturnogo materialovedeniya. Vozmozhnosti i problemy [Fundamentals of nanostructured materials science. Opportunities and challenges]. Moscow: BINOM. Knowledge Laboratory. 252 p.
  21. Dmitriev, A. S. 2021. Vvedenie v nanoteplofiziku [Introduction to nanothermophysics]. Moscow: BINOM. Knowledge Laboratory. 790 p.
  22. Maldovan, M. 2013. Sound and heat revolutions in phononics. *Nature* 503:209–217.
  23. Zhmakin, A. I. 2021. Heat conduction beyond the Fourier law. *Tech. Phys.* 66(1):1–22. doi: 10.1134/S1063784221010242.
  24. Morozov, A. I., and A. S. Sigov. 1994. Kinetic phenomena in metals with quantum defects. *Phys. — Usp.* 37(3):229–247. doi: 10.1070/PU1994v037n03ABEH000010.
  25. Klimontovich, Yu. L. 1995. *Statistical theory of open systems*. Dordrecht: Kluwer Academic Publs. Vol. 1. 412 p.
  26. Zubarev, D., V. Morozov, and G. Röpke. 1996. *Statistical mechanics of nonequilibrium processes. Vol. 1: Basic concepts, kinetic theory*. Physical research ser. Berlin: Akademie Verlag. Vol. 21. 375 p.
  27. Leontovich, M. A. 1935. Osnovnye uravneniya kineticheskoy teorii gazov s točki zreniya sluchaynykh protsessov [Basic equations of the kinetic theory of gases from the viewpoint of random processes]. *ZhETF* [J. Exp. Theor. Phys.] 5(3–4):211–231.
  28. Kolmogorov, A. N. 1931. Über die analytischen Methoden in der Wahrscheinlichkeitsrechnung. *Math. Ann.* 104:415–458.
  29. Pleshivtsev, N. V., and A. I. Bazhin. 1998. *Vspuchivanie i shelushenie poverkhnosti (blistering i fleking)* [Swelling and peeling of the surface (blistering and flecking)]. Moscow: Vuzovskaya kniga. 392 p.
  30. Kukushkin, S. A. 2003. Nachal'nye stadii khрупkogo razrusheniya tverdykh tel [Initial stages of brittle fracture of solids]. *Uspekhi mekhaniki* [Advances in Mechanics] 2(2):21–43.
  31. Bondareva, A., G. Zmievskaia, and T. Levchenko. 2014. Radiation damage thin coating of silicon carbide. *J. Phys. Conf. Ser.* 510:012010. doi: 10.1088/1742-6596/510/1/012010.
  32. Averina, T. A., and S. S. Artem'ev. 1986. A new family of numerical methods for solving stochastic differential equations. *Soviet Mathematics Doklady* 33(3):736–738.
  33. Skorokhod, A. V. 1965. *Studies in the theory of random processes*. Reading, MA: Addison-Wesley Publishing Co., Inc. 199 p.
  34. Krylov, N. V. 1972. An inequality in the theory of stochastic integrals. *Theor. Probab. Appl.* 16(3):438–448. doi: 10.1137/1116049.
  35. Krylov, N. V. 1980. *Controlled diffusion processes*. Transl. A. B. Aries. Applications of mathematics ser. New York, Berlin: Springer-Verlag. Vol. 14. 308 p. doi: 10.1007/978-1-4612-6103-2.
  36. Zmievskaia, G. I., and A. L. Bondareva. 2012. Chislennoe modelirovanie kinetiki vzniknoveniya poristosti v mnogosloynnykh sredakh [Numerical simulation of the kinetics of porosity occurrence in multilayer media]. *Fizicheskie i matematicheskie modeli plazmy i plazmopodobnykh sred* [Physical and mathematical models of plasma and plasma-like media]. Eds. D. Maino and G. Zmievskaia. Moscow: Keldysh Institute of Applied Mathematics RAS. 16–27. Available at: <https://keldysh.ru/papers/2012/article/ZmiMaino-label.pdf> (accessed February 22, 2026).
  37. Norman, G. E., and V. V. Stegailov. 2011. Metod klassicheskoy molekulyarnoy dinamiki: zamysel i real'nost' [Classical molecular dynamics method: Concept and reality]. *Nanostrukturny. Matematicheskaya fizika i modelirovanie* [Nanostructures. Mathematical Physics and Modelling] 4(1):31–58.
  38. Zmievskaia, G. I. 2020. Stochastic model of pore nucleation during sample irradiation with inert gas ions. *Mech. Solids* 55(1):132–141. doi: 10.3103/S002565442001018X.
  39. Zmievskaia, G. I. 2019. Computer simulation of phase transition nonequilibrium processes. *Nonequilibrium processes*. Eds. S. M. Frolov and A. I. Lanshin. Moscow: TORUS PRESS. 1:118–126.
  40. Bondareva, A. L., and G. I. Zmievskaia. 2010. Simulation of blistering in layered mirrors used in lithography. *J. Surf. Invest. — X-ray* 4(3):415–424. doi: 10.1134/S102745101003006X.

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