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Structure-dynamic approach of nanoionics. Theory and computer exploration.

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Abstract content
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We have put forward structure-dynamic approach (SDA) [1,2] for computer modeling of the dynamic behavior of solide electrolyte (SE) nanosystems with fast ionic transport (FIT) and for the further development of nanoionics [3]. Theoretical system of SDA includes a structural layered 1D-hopping atomic model of the region with a non-uniform potential landscape, a method of "hidden" variables (excess concentrations of mobile ions induced by external influence on crystallographic planes), a physico-mathematical formalism (based on the principle of a detailed balance and the kinetic equation in the form of the particle conservation law), and a method of uniform effective field. A new notion - the Maxwell displacement current on a potential barrier and the essential definition of effective electrostatic field (corrected uniform Gauss field) [2,4] are given. The computer exploration (in the "Wolfram Mathematica" package) of the ion-transport and dielectric-polarization processes of model SE nanosystems are analyzed, and such modes of solid state ionics as "near constant loss" and Johnsher's universal dynamic response (the power law of the real part of frequency dependent conductivity) are explained. The results of this work will help to overcome certain problems, which hinder development of the perspective matrix devices with FIT at the nanoscale level, such as memory cells with SE-programmed metallization, supercapacitors of micron sizes with a record high density of energy and charge, field effect transistors with SE gates, sensors and memristors.

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[2] A.L. Despotuli, A.V. Andreeva. Ionics 21 (2015) 459.
[3] A.L. Despotuli, V.I. Nikolaichik. Solid State Ionics. 60 (1993) 275.
[4] A.L. Despotuli, A.V. Andreeva. Ionics 22 (2016) DOI 10.1007/s11581-016-1668-3

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