SIMULATION OF DELAY REACTION-DRIFT-DIFFUSION SYSTEM APPLIED TO CHARGING EFFECTS IN ELECTRON-IRRADIATED DIELECTRICS

A. Maslovskaya, A. Pavelchuk

**Department of Mathematics and Computer Sciences, Amur State University,
21 Ignatyevskoe Shosse, Blagoveshchensk 675000, Russia**

Abstract. The paper presents the results of mathematical modeling of reaction-convection-diffusion type system with time delay and its application to numerical simulation of charging process in dielectrics irradiated by electron bunches with average energies.
The mathematical model was expressed in the form of mixed initial-boundary value problem for generalized reaction-convection-diffusion equation in several space dimensions with permanent time delay. An advanced finite difference scheme was suggested to numerically solve the delay parabolic PDE. The modification of computational splitting scheme was based on alternating direction method of Peacman-Rachford for approximation of "diffusion" part of PDE as well as Roberts-Weiss scheme was used for approximation of "convection" part of PDE. In order to approximate the "reaction" part of PDE the "frozen coefficient" method was also applied. The procedure of approximation analysis resulted in second order accuracy for space as well as time variables. The stability analysis by means of maximum principle allowed us to specify the absolute stability of the scheme. The constructed numerical scheme was modified taking into account delay effect. The main peculiarity of delay system numerical simulation is necessity of memory-stored control for delay "window" structure (values of decision variable on each time layer including to delay period). This aspect leads to resource-intensive computational process.
The proposed algorithm was included into the general hybrid computational scheme to simulate dynamic charging process in dielectrics irradiated by electron beam. This effect can be observed at diagnostics and modification of such materials with use of scanning electron microscope techniques. The mathematical model of dielectric charging involves locally instantaneous Poisson equation and time-dependent transport equation. The latter is reaction-drift-diffusion equation in several space dimensions with time delay. Monte-Carlo simulation of electron transport in electron irradiated target was also used to estimate a source function. The special program application developed with Matlab package was designed to simulate dynamic electron beam-stimulated charging processes in dielectrics. Three modes of charging process were implemented in the program: the stationary mode, the dynamic mode of charge relaxation and the dynamic mode of charge accumulation. The relation of deposits of "drift" (convection) and "diffusion" parts in the model for dynamic modes was also discussed using analysis of value of Peclet number. The computing experiments by the example of ferroelectric crystal were performed to estimate the charge density distribution, potential distribution as well as field intensity electron beam-induced.

Keywords: reaction-convection-diffusion equation, delay parabolic PDE (partial differential equation), splitting method, electron beam irradiation, charging of dielectrics, mathematical model of charging process, simulation of charging characteristics