Fractal model of polarization switching kinetics in ferroelectrics under nonequilibrium conditions of electron irradiation

A G Maslovskaya and T K Barabash
Mathematics and Computer Science Department, Amur State University, 21 Ignatyevskoe Shosse, Blagoveshchensk, 675000, Russia
E-mail: maslovskayaag@mail.ru

Abstract. The paper presents the results of the fractal and multifractal analysis of polarization switching current in ferroelectrics under electron irradiation, which allows statistical memory effects to be estimated at dynamics of domain structure. The mathematical model of formation of electron beam-induced polarization current in ferroelectrics was suggested taking into account the fractal nature of domain structure dynamics. In order to realize the model the computational scheme was constructed using the numerical solution approximation of fractional differential equation. Evidences of electron beam-induced polarization switching process in ferroelectrics were specified at a variation of control model parameters.

1. Introduction
Presently the study of nonequilibrium processes in complex physical systems becomes one of the major scientific directions which widely use the methods of mathematical modelling and computer simulation. In particular, the well-known examples of simulated process in such systems include the nonequilibrium dynamics, phase transitions and domain kinetics in ferroelectric materials. Ferroelectrics are related to the promising subclass of polar dielectrics, which have a wide range of applications in microelectronics, optoelectronics, acoustics, radio engineering, piezo- and pyrotechnics due to polarization switching under external exposure. The numerous studies have been devoted to theoretical and experimental justifications of the domain boundaries movement, restructuring of domain configurations and kinetics of polarization switching in ferroelectrics. These findings have also indicated that domain structures reveal fractal properties and self-similar behavior [1-5].

In order to describe the quantitative characteristics of self-organization processes in complex physical systems the methods the fractal theory can be used [6]. The concept of a fractal is geometrical one and it sets the self-similar object which can be described by fractal dimension. However, not only the geometrical forms of objects can have a fractal structure but also dynamic characteristics of the processes and the phenomena also can find the self-similar behavior in materials with self-similar structure [7-8].

Previous works have shown that the self-similarity property of ferroelectric domain structure is not the only fractal characteristic of ferroelectrics. Dynamic characteristics of ferroelectrics demonstrate fractal properties likewise [9-11]. Indeed, the methods of fractal and multifractal analysis of time series can be effectively used to study the scaling characteristics of polarization switching of process in ferroelectrics.
Notice that the methods of fractal analysis allow us to identify only a posteriori estimates of physical process characteristics. So as to construct the mathematical model of physical system dynamics traditionally one can use the ordinary or partial differential equations. Nevertheless such approach cannot provide model adequacy for many objects and processes which possess self-similarity properties. The application of concepts of the fractional differential calculus theory is the relevant aspect of mathematical models modification to describe the behavior of fractal physical systems. In this case, to formalize the memory processes and phenomena one can employ a time fractional derivative. In addition, space fractional derivatives enable us to take into account the fractal properties of the material inhomogeneity [12-13].

The diagnostics of domain structure as well as modification of electrical properties of ferroelectrics can be performed using scanning electron microscope (SEM) techniques [14-17]. In particular, the application of the electron beam stimulated polarization current mode allows us to visualize SEM-contrast of ferroelectric domains and simultaneously to observe the process of polarization switching [17]. The main dynamic characteristic of polarization switching process is determined by the video signal which is electric response of ferroelectric sample. The polarization switching current is represented as time dependence which is attributed to intensity of the polarization processes in a crystal. Therefore the specific character of this problem requires developing of the theoretical justification. This allows us to formalize observed processes, to investigate scaling characteristics of polarization switching process in ferroelectrics and to predict behavior of system based on computing experiments [18]. The following study was undertaken to develop the mathematical model of electron beam stimulated polarization switching in ferroelectrics taking into account the results of fractal and multifractal analysis of polarization current registered in the injection mode.

2. Fractal and multifractal analysis of dynamic characteristics of polarization switching in ferroelectrics under electron irradiation

Fractal regularities of dynamic characteristics behavior are due stochasticity of nucleation process in ferroelectrics, nonlinear reorganization and dynamics of the domain structure, existence of defect structure as well as memory effects which, in particular, are shown by repeatability of the nucleation centers at cyclic of polarization switching. In this notation, nonlinear dynamics of domain structure is caused by lateral or through domain growth during polarization switching process and interaction of domain boundaries with defects notably pinning.

To be definite, assume that the object of fractal analysis is set to be time dependence of polarization switching currents in typical ferroelectric crystal TGS ((NH₄)₂H₂PO₄, triglycerine sulfate) registered with the electron beam-stimulated polarization current mode [17]. The study was based on methods of fractal and multifractal analysis.

The Hurst method (so-called rescaled range analysis or R/S-analysis) and Fourier method were applied to estimate fractal dimension of polarization switching current represented as time series [6]. The Hurst method includes the following steps. First time series is splitting into non-overlapping segments \( I_n \) of size \( n \). Then, the integrated term is calculated in each segment and the local trend is also estimated. Secondly the rescaled range is averaged over all segments with respect to \( n \) and the Hurst exponent \( H \) can be obtained using the following equation:

\[
\left( \frac{R}{S} \right)_n = \frac{1}{A} \sum_{a=1}^{A} \frac{R_{I_a}}{S_{I_a}} \propto n^H ,
\]  

(1)

where \( R_{I_a} = \max \{X_{k,a}\} - \min \{X_{k,a}\} \) is maximum value of the range; \( X_{k,a} \) is time series of accumulated deviations from average value for each period \( I_a \); \( S_{I_a} \) is standard deviations calculated for each period \( I_a \).

The angular coefficient of linear approximation of functional dependence (1) by least-squares procedure in log-log scale is determined by Hurst parameter \( H \) and fractal dimension \( D = 2 - H \).
Generally three various dynamics depending on Hurst parameters are usually considered. While value $0 < H < 0.5$ indicates long-term anti-correlated behavior of the data; $H = 0.5$ corresponds to the random and uncorrelated events; $0.5 < H < 1$ is referred to as persistent series and the trending stability of behavior increases as long as $H$ tends to the unit.

In addition, Fourier method was used to estimate the fractal parameters [6]. This method is based on Fourier transform. The procedure of Fourier decomposition of time series $y(t)$ permits us to obtain the values of amplitude $c$ and phase $\varphi$ for some fixed number of frequencies $f$:

$$y(t) = \sum_{f = f_{\text{min}}}^{f_{\text{max}}} c(f) \cdot \sin\left(2\pi \cdot f \cdot t + \varphi(f)\right).$$

(2)

Therefore, the fractal dimension $D$ of time series can be evaluated provided we calculate the power spectral density $c^2(f)$. Using the following relation $c^2(f) \sim f^\beta$ and linear approximation of $c^2(f)$ with double log scale we also can estimate the angular coefficient $\beta$ related to fractal dimension according to the expression $D = (4 + \beta)/2$.

Moreover, the methods of multifractal analysis can be more informative techniques used to study scaling characteristics of dynamic data at diagnostics of physical systems. The multifractal methods are perspective tools used to research of complex systems behavior. This allows to determine a continuous spectrum of fractal dimensions $f(\alpha)$ and to localize time as well as scale properties of time series. In this study, the method of multifractal detrended fluctuation analysis (MDFA) [7] and the wavelet transform maxima modules method (WTMM) [8] were implemented.

The MDFA procedure is based on the following principles [7]. At the first step initial time series $y_k(t_k)$ of length $N+1$ is transformed into a new series using the equation $z_i(x_i) = \ln(y_{i+1} / y_i), i = 1,N$. After that, a profile is specified as $x_j = \sum[z_i - \bar{z}], i = 1,j, j = 1,\bar{N}$, where $\bar{z}$ is the mean of series $z$.

Then $x_j$ is splitting into $N_s = \text{int}(N/s)$ nonoverlapping segments of equal length $s$. It follows that the local trend and variance $F^2(v,s)$ are determined for each of the $2N_s$ segments lengthwise the forward and reverse directions. Then the average over all segments is calculated to obtain the $q$-th order fluctuation function:

$$F_q(s) = \left[\frac{1}{2N_s} \sum_{v=1}^{2N_s} \left[F^2(v,s)\right]^{q/2}\right]^{1/q} \propto s^{h(q)}.$$

(3)

Finally, fluctuation function $F_q(s)$ is analyzed using logarithmic scales. Multifractal scaling exponents $\tau(q)$ are determined by formula $\tau(q) = qh(q) - 1$. Also the singularity spectrum $f(\alpha)$ and singularity strength $\alpha$ related to $\tau(q)$ characterize a multifractal series via Legendre transformation according to the following equations:

$$\alpha = \tau'(q), \quad f(\alpha) = q\alpha - \tau(q).$$

(4)

Further, WTMM uses the wavelet transform with continuous basis soliton-like functions. Here the local extremum lines of a surface of wavelet coefficient $W(a,b)$ for each scale $a$ are calculated. Then partial functions $Z(q,a)$ are evaluated as:

$$Z(q,a) = \sum_{l \in L(a), a', a' \leq a} \left(\sup_{a'} W(a',b_l(a'))\right)^q \propto a'^{\tau(q)}, \quad W(a,b) = (1/a) \int_{-\infty}^{\infty} x(t) \psi((t-b)/a) dt,$$

(5)
where $W(a,b)$ is the continuous wavelet transform of function $x(t)$; $a$ is a scale, $b$ is a time position, \(\psi\) is a mother wavelet (in particular, “Mexican hat” wavelet was used); the largest value of the wavelet transform coefficients modules is selected along each line on scales less then $a$, $L(a)$ is a set of all ($l$) local maxima lines of wavelet transform modules existing on scale $a$, $x_l(a)$ is the line maximum $l$ position on the scale $a$. The scaling exponents $\tau(q)$ characterize the multifractal properties related to singularity spectrum $f(\alpha)$ obtained by Legendre transformation.

The program application realizing the methods of fractal and multifractal analysis was suggested to perform computing experiments. The software was designed using program application package Matlab. The structure of program application is shown in figure 1.

![Program application structure](image)

**Figure 1.** Program application structure for fractal and multifractal analysis of time series.

Program verification was performed using the generated time series with a priori specified fractal dimension. Hurst method allows us to obtain the result with accuracy order 0.001 while Fourier method is less exact and it has the order of accuracy of 0.01.

The Figure 2 (a) demonstrates the fractal characteristics calculated for time dependence for polarization switching current in TGS crystal registered with injection mode of SEM.

![Figure 2](image)

(a)

**Figure 2.** The result of $R/S$-analysis – (a); the singularity spectrum $f(\alpha)$ calculated by MDFA and the image of wavelet coefficient surface calculated by WTMM – (b) for polarization switching current in TGS (displayed in the insert figure).
The computed characteristics lead to the following results. Hurst parameter equals to \( H = 0.73 \) and the corresponding value of fractal dimension is going to be \( D = 1.27 \). This finding suggests the self-similarity organized movement of domain boundaries during the polarization reversal processes in ferroelectric crystals under external exposure.

Fractal behavior of domain structure dynamics can be characterized by persistent features due to effects of long-term memory. The polarization reorientation observed in ferroelectrics under electron beam irradiation is not actually a random process. This means that previous positions of domain boundaries impact the process of the formation of subsequent positions.

The results of multifractal analysis performed using multifractal detrended fluctuation analysis and the wavelet transform maxima modules method are presented in figure 2 (b). The image of wavelet coefficient surface demonstrates hierarchical arrangement of polarization current fluctuations referred to domain restructuring. This feature is caused by the fact that the observable signal has self-similarity properties. The calculated spectrum of fractal dimensions exhibits a variation of fractal dimension values over the range \( 0.9 \leq D \leq 1.9 \), which confirms the assumption of the multifractal nature of polarization switching process in ferroelectrics exposed to electron irradiation. The maximum abscissa of a spectrum curve corresponds to Hurst parameter of fractal process. We may assume that the fractal characteristics specify characteristic dimension of kinetic process. Hence, scaling characteristics identified by fractal analysis methods can be used for mathematical model construction to describe the polarization switching process in ferroelectrics irradiated by electron beam.

3. Experimental aspects of polarization switching kinetics in ferroelectrics and conceptual problem definition

In order to formalize the electron beam-induced reorientation of domain structure in ferroelectrics we accepted a number of assumptions. Let us consider the evolution of 180° ferroelectric domains. To be definite also we assume that electron beam injection into sample on the depth of \( I \) results in accumulating charge with surface charge density \( \sigma \) in the irradiated layer and charges with surface charge densities \( \sigma_1 \) and \( \sigma_0 \) on the top and bottom electrodes respectively. By turn this induces the occurrence of the electric fields \( E_1 \) in the irradiated layer and \( E_2 \) in the main volume of material. The field intensity \( E_2 \) can activate polarization switching processes in domains “tail-to-beam” orientated and, in the converse case, it can stabilize the domain structure with “head-to-beam” orientation of spontaneous polarization vector \( P_s \) as shown in figure 3.

**Figure 3.** The diagram of domain growth (\( I \) is electron injection depth, \( x \) is instant position of domain boundary; \( z \) is corresponding average instant position of domain boundary).

To describe the main dynamic characteristics of process, which is given by polarization switching current, we use the general equation known as Kolmogorov-Avrami model [19-21]. In compliance with this approach the polarization current is expressed by a relation of the switched volume to the total volume of a crystal. In our case we suggest to modify this equation using the dependence of domain boundary velocity \( v \), which is transformed to the formula:

\[
I(t) = \frac{2P_S S}{L} \frac{dx}{dt}, \quad v = \frac{dx}{dt} = v_\infty \exp \left( -\frac{\delta}{E_2} \right),
\]  

(6)
where $L$ is sample thickness in m; $v_\infty$ is maximum value of domain boundary velocity at $E \to \infty$ in m/s; $\delta$ is activation field in V/m; $S = 2\gamma d$ is irradiated area in m$^2$.

In view of the importance of polarization switching process in the electron beam polarization current mode, let us assume the following mechanisms of domain growth. The polarization switching is realized by means of growth of domains with wedgewise form with the fixed width of the base $2y$ and the changing angle of domain boundary slope $\phi$. The geometrical scheme of domains growth is shown in figure 4.

![Figure 4](image)

Figure 4. The geometrical scheme of sequential stages of growth of wedgewise domains.

The polarization switching process is going to be completed as long as the middle of wedge $z(t) = l + x(t)/2$ reaches the boundary of crystal $L$. The use of such mechanism permits us to specify falling of the polarization current at completion of polarization switching process.

4. Mathematical model: fractal approach

The evidences caused by fractal analysis of polarization current in ferroelectrics confirm that the reorganization of domain structure demonstrates a complex scaling behavior. In this terms polarization switching process can be characterized by long-term memory effect. Reorientation of domains polarization has nonrandom character provided the formation of the subsequent conditions based on the previous states of domain structure. Note also that the agreement of simulation results with experiment data can be observed if one uses the modified Kolmogorov-Avrami models with fractional values of kinetic process dimension [5], [10], [20], [21].

We applied fractional differential calculus to describe the domain boundary dynamics at switching polarization as fractal process with power-series memory. The fractal nature of the movement of domain boundaries can be under consideration using a fractional order derivative with respect to time. Therefore, we express the equation defining the polarization switching process (6) subjected to a dimensionless form with use of fractional differentiation operator. After some transformations we can rewrite the equation of domain dynamics in the following form:

$$\frac{d^\alpha s}{dw^\alpha} = \exp\left(-\tau_2 \left[\frac{\tau_3 w + \tau_3}{2l} \left(1 + \cos^2 \phi \frac{L_s}{2} \right) \right]^{-1}\right), \quad s(w_0) = 0, \quad 0 \leq s(w) \leq 2(1 - l/L), \quad (7)$$

where $s = x/L$ and $w = t/\tau_1$ are dimensionless distance and time variables; $\alpha$ is the dynamic fractal dimension varied over the range of $(0.5, 0.99)$; $\cos^2 \phi = y^2 / (x^2 + y^2)$; $\tau_1 = L/v_\infty$ is the characteristic time of boundary growth through a crystal in s; $\tau_2 = \delta \epsilon_0 L/(jl)$ is the characteristic time of accumulation of charge generating the field $E_2 = \delta$ at given current density $j$ (in $A/m^2$) in s; $\delta$ is activation field in V/m; $\tau_3 = 2P_3/j$ is the characteristic time period during which the charge density $\sigma$ is defined to be $2P_3$ in s.

The expression for the field $E_2$ in unirradiated part of sample was used in general equation (7) in the following form:
\[ E_2(w) = \frac{j\tau w}{\varepsilon_0 L} + \frac{P_s}{\varepsilon_0 L} \cdot \frac{L}{2} \left(1 + \cos^2 \varphi\right). \]  

The formula (8) was determined taking into account the effect of boundary profile bending which is formed during domain boundary moving. Furthermore we can express the polarization switching current as follows:

\[
I(w) = \begin{cases} 
4 \cdot P_s \cdot \frac{d^2y}{d\omega \gamma} \cdot \frac{d^2s}{d\omega \gamma}, & \text{if } 0 \leq s \leq 1 - \frac{l}{L}, \\
4 \cdot P_s \cdot \frac{d^2y}{d\omega \gamma} \cdot \frac{L^2}{s^2} \cdot \frac{1 - \frac{k}{M}}{d\omega}, & \text{if } 1 - \frac{l}{L} \leq s \leq \frac{1 - (1 - \frac{l}{L})}{2}.
\end{cases}
\]  

where wedge basis \( y \) is splitting into \( M \) number of discrete intervals, \( k = 0, M \).

Indeed, the polarization switching process is attributed to growth of \( n \) wedge-shaped domains with an identical speed and width of the base \( 2y/n \). The polarization current is determined by superposition of deposits which are given by separate switching areas.

As a result, model of polarization switching current and domain dynamics includes the initial value problem for the fractional differential equation (7), expressions for the field intensity (8) and switching current (9). To obtain the dependences \( I(t) \) and \( E_2(t) \) one needs to execute the inverse change of variable \( t = w \cdot \tau_1 \).

5. Numerical scheme of model implementation

The problem (7) can not be solved by analytical methods and requires using numerical procedures. The numerical scheme was constructed to solve the fractional differential equation. The Grunwald-Letnikov definition provides a convenient finite difference discretization of fractional derivative operators [12-13]. To approximate the fractional derivative of \( p \) with respect to variable \( \xi \) the Grunwald-Letnikov formula was used [22]:

\[
\frac{d^n p(\xi)}{d\xi^n} = \lim_{h \to 0} \frac{1}{\Gamma(-\alpha)} \cdot \frac{1}{h^n} \cdot \sum_{i=0}^{\infty} \frac{\Gamma(i-\alpha)}{\Gamma(i+1)} p(\xi - ih),
\]

where \( h \) is time step; \( \Gamma(\alpha) \) is the gamma function.

The fractional derivative is nonlocal convolution type operator. This implies that the value of a fractional derivative with time depends on function values at all previous time moments. Thus, the value of function is defined by all previous states in each time moment. Sequential approximation of a fractional derivative for each element \( i \) on a grid \( \Omega = \{w_i = w_0 + ih, i = 0, N\} \) can be expressed in the following form:

\[
\frac{1}{\Gamma(-\alpha)} \cdot \frac{1}{h^n} \left( \frac{\Gamma(\alpha)}{\Gamma(1)} s_1 + \frac{\Gamma(1-\alpha)}{\Gamma(2)} s_0 \right) = f(s_0, w_0), i = 1;
\]

\[
\frac{1}{\Gamma(-\alpha)} \cdot \frac{1}{h^n} \left( \frac{\Gamma(\alpha)}{\Gamma(1)} s_2 + \frac{\Gamma(1-\alpha)}{\Gamma(2)} s_1 + \frac{\Gamma(2-\alpha)}{\Gamma(3)} s_0 \right) = f(s_1, w_1), i = 2;\
\]

where \( f(s, w) \) is right hand side of differential equation (7).

Hence, explicit numerical scheme can be written in the form:
\[ s_{i+1} = \Gamma(1) \left[ h^D f (s_i, w_j) - \sum_{j=1}^{i+1} A_j^D s_{i-j+1} \right], \quad A_j^D = \frac{\Gamma(j-\alpha)\Gamma(-\alpha)\Gamma(j+1)}{\Gamma(-j)} . \] (11)

The general scheme (11) demonstrates the main idea of fractional derivative used to simulate physical system with memory effect. This means that to simulate the self-similar domain boundary dynamics previous provisions time depended are taken into account.

6. Initialization of simulation parameters

To implement a computing experiment we have to specify a set of the parameters corresponding to physical experiment. Simulation of polarization reversal processes was performed with respect to ferroelectric crystal TGS which can be switched under the conditions of electron beam irradiation [17]. Geometrical parameters of a sample were set to be the following: \( L = 10^{-3} \text{ m} \) is thickness of a crystal; \( S = 0.25 \cdot 10^{-6} \text{ m}^2 \) is the irradiated area on the top electrode of a sample; the linear sizes of the irradiated area are correspond to \( d = 2y = 0.5 \cdot 10^{-3} \text{ m} \) (the base of switching area is splitting into \( n = 20 \) elements).

Physical parameters were also defined. Let us specify the dielectric permittivity \( \varepsilon = 50 \), electric constant \( \varepsilon_0 = 8.85 \cdot 10^{-12} \text{ F/m} \). The spontaneous polarization is equal to \( P_s = 2 \cdot 10^{-2} \text{ C/m}^2 \) for TGS crystal. Time characteristic parameters were estimated to be \( \tau_1 = 13.5 \text{ s} \), \( \tau_2 = 37 \text{ s} \), \( \tau_3 = 16.5 \text{ s} \), which correspond to value of the activation field \( \delta = 6 \cdot 10^5 \text{ V/m} \) and injection current density \( j = 2.4 \cdot 10^{-3} \text{ A/m}^2 \) at probe current \( I = 6 \cdot 10^{-10} \text{ A} \).

Thickness of injection layer \( l \) was determined using the results of Monte Carlo simulation of electron transport in irradiated target [23-24]. As an example the result of computer simulation of electron trajectories for TGS crystal at start beam energy \( E_0 = 15 \text{ keV} \) is shown in figure 5. Here we retraced \( N = 10000 \) stories of electrons.

![Figure 5. The result of Monte-Carlo simulation of electron trajectories for TGS crystal.](image)

Note that Monte Carlo simulation of electron injection for ferroelectrics coated by metal (silver, aluminum or gold) electrodes at the same value of start beam energy leads to similar geometry of electron interaction zone with material. In this case, the thickness of an electrode should be smaller than \( 1 \mu \text{m} \). In this way, the electrons can freely penetrate into the sample and accumulate in surface layer. This creates the necessary condition to start polarization switching process in ferroelectrics in injection mode of SEM. The trajectories visualized by dark color are correspond to transmitted electrons while
emitted trajectories are visualized by light color. The depth of electron injection is approximately equal to \( l \approx 3 \mu m \).

7. Computing experiments and discussions

The model (7)-(9) was implemented using the numerical algorithm (11). Verification of computer simulation results was performed in two steps. First, simulation data was compared to analytical solutions for test problems which were presented in the form of initial problem for fractional differential equations. Secondly, we established a numerical convergence of calculation results obtained with the scheme (11) (at the fractal parameter \( \alpha = 0.99 \)) and the results of determinate model calculated by predictor-corrector Adams methods of third-order accurate.

The results of fractal and multifractal analysis of polarization switching current in TGS allow us to conclude that Hurst parameter complies the fractal parameter \( \alpha \) in the model of polarization current formation (7)-(11). Therefore, we can assume that fractal parameter \( \alpha \) as a scaling parameter of domain dynamics can be calculated in terms of fractal and multifractal methods.

The figure 6 \( a \) represents the simulation result of switching current impulse compared to experimental curve (calculation is performed at given above parameters and fractal parameter is set to be 0.73). The curve of polarization switching current reproduces peculiarities experimentally observed (when signal is recorded with the bottom electrode). The following features can characterize the impulse of polarization switching current in TGS crystal. The curve of switching current has the "peaked" maximum, which is characteristic for a pulse mode of SEM. The polarization current impulse has the duration of tens of seconds and the total charge of polarization reversal corresponds to the relation \( 2P_0 \cdot S \). The processing of data presented in figure 6 \( a \) gives the estimation of standard deviation of model from experimental curve equal to \( 5 \cdot 10^{-11} \).

The figure 6 \( b \) illustrates time dependence of domain boundary dynamics. The start time required to accumulate a charge and also to begin the switching process is estimated to be \( t_{st} = 8 \) s. During the process observation \((42 - 45)\) s the domain boundary reaches the bottom electrode when the switching process is finished and the main volume of a crystal will be characterized by inverse value of a vector \( P_s \).

![Figure 6](image)

**Figure 6.** The model representation of polarization switching current in TGS \((I)\) compared with experimental data \([17]\) (2) – (a); time dependence of coordinate of domain boundary (the curve \( I \) is corresponded to fractal model, the curve 2 displays the result obtained with determinist model) – (b).

The comparative analysis of the curves calculated by means of fractal and deterministic models indicates that domain dynamics has complex character. Domain boundary movement can be characterized by non-linear behavior compared with almost linear growth of \( x(t) \) in of the deterministic model. This is caused by memory effect occurrence in physical system.
Variation of the control parameters allows modelling main characteristics of domain structure switching related to conditions of experimental observation. The start time $t_{st}$ of polarization switching process in TGS as a function of injection current density $j$ (change in parameters $\tau_3$ and $\tau_2$ depending on $j$) for seven realization of model is shown in figure 7.

![Figure 7](image)

**Figure 7.** The start time of polarization switching as a function of injection current density for TGS (approximation by exponential relationship).

Also we can conclude that the character of model behavior corresponds to experimentally observed regularities of process. Here start time of polarization switching process decreases exponentially from 24 s to 4 s when injection current density increases from $0.9 \cdot 10^{-3}$ A/m$^2$ to $5 \cdot 10^{-3}$ A/m$^2$.

### 8. Conclusions

Thus, fractal and multifractal analysis of electron beam-induced polarization switching currents in ferroelectrics represented as time series was performed. The analysis was based on Hurst method, Fourier method as well as multifractal detrended fluctuation analysis and the wavelet transform maxima modules method. The fractal dimension, Hurst parameter, scaling exponents, singularity spectrum were calculated. The calculated spectrum gives a variation of fractal dimension in the wide range. The image of wavelet coefficient surface demonstrates hierarchical arrangement of polarization current fluctuations. These results suggest that domain structure reorganization demonstrates the complex self-similar nature. The dynamics of polarization switching process can be characterized by effect of statistical memory and formation of the subsequent conditions is based on previous states during domain reorientation process. Software application was developed to support fractal and multifractal analysis of complex signals.

The present study also demonstrates that characteristics specified by fractal analysis can be used to simulate the polarization switching process in ferroelectrics. The mathematical model of polarization switching in the injection mode was presented. The model permits us to simulate polarization current formation taking into account fractal nature of domain dynamics. The model is expressed by the initial problem for fractional differential equation describing the domain boundary movement as well as expression for calculation of polarization switching current.

The computational algorithm was proposed to realize this model. The numerical scheme was based on numerical approximation of fractional derivative by the Grunvald-Letnikov formula. Model calculation of polarization switching current in TGS crystal was implemented under the conditions corresponding experiment data in injection mode of SEM. The model reproduces correctly the main features of observed polarization switching currents in TGS. Computing experiment allows identifying characteristics of polarization switching kinetics depending on a variation of control scanning parameters in SEM, which are probe current and the accelerating voltages.
References

[1] Galiyarova N and Donysova L 1999 Ferroelectrics 222 269
[2] Ozaki T, Fujii K and Ohgami J 1995 J. Phys. Soc. Jpn. 64 2282
[3] Wu Z, Duan W, Wu J and Gu B-L 2007 Nanotechnology 18 325703
[4] Roy M K, Paul J and Dattagupta S 2010 IEEE Xplore 109 014108
[5] Scott J F 1998 Fractal dimensions in switching kinetics of ferroelectrics (Cambridge: University of Cambridge Press) p 9
[6] Bojokin S V and Parshin D A 2001 Fractals and multifractals (Moscow: R&C Dynamics)
[7] Kantelhardt J W Fractal and multifractal time series (Halle-Wittenberg: Institute of Physics, Martin-Luther-University) p 42
[8] Pavlov A N and Anishchenko V S 2007 Physics of the Solid State 44 2151
[9] Mateos L, Bausa L E and Ramirez M O 2013 Applied Physics Letters 102 042910
[10] Ishibashi Y 1990 J. Phys. Soc. Jpn. 59 4158
[11] Meilanov R P and Sadykov S A 1999 Technical Physics 44 595
[12] Zhang Y, Zhong X L, Zhang Z H, Wang J B and Zhou Y C 2012 Proc. SPIE 8409 84091Q
[13] Scherer R, Kallab S L, Tange Y and Huang J 2011 Computers & Mathematics with Applications 62 902
[14] Joy D C 1995 Monte-Carlo modeling for electron microscopy and microanalysis (New York: Oxford University Press) p 216
[15] Demers H, Poirier-Demers N, Couture A R, Joly D, Guilmain M, de Jonge N and Drouin D 2011 Scanning 33 135