INTERNATIONAL CONFERENCE
DAYS ON DIFFRACTION

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Session: Numerical approac

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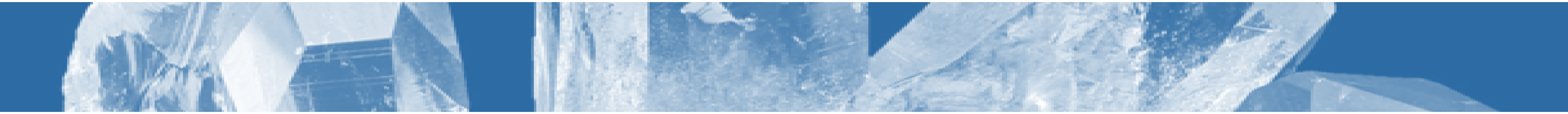

COMPUTATIONAL TECHNIQUES FOR TIME-FRACTIONAL MODELLING OF THERMAL WAVE PROPAGATION IN FERROELECTRICS

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OUTLINE

- ✓ INTRODUCTION & MOTIVATION
- ✓ TIME-FRACTIONAL MODEL OF THERMAL WAVE PROPAGATION IN FERROELECTRICS
- ✓ COMPUTATIONAL SCHEME & IMPLEMENTATION OF NUMERICAL ALGORITHM
- ✓ COMPUTATIONAL EXPERIMENTS
- ✓ SUMMARY

INTRODUCTION & MOTIVATION

ECTS

Dielectrics

Piezoelectrics

Pyroelectrics

Ferroelectrics

roelectric emories, FRAM

Electrooptic & Acoustooptic Devices

Pyroelectric Devices, Infrared Sensors, Vidicons

Vave uides

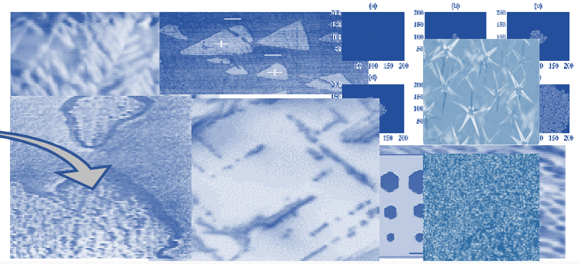
Sensors, Actuators, Filters, Vibrators, SAW elements, Transformers

NLO Devices, Optical Modulators

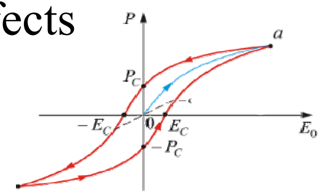
Selected applications of ferroelectrics

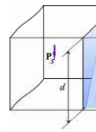
e elements in microelectronic devices, pyroelectric cs, optoelectronics, microprocessor technologies, …)

FERROELECTRICS



- a class of promising dielectrics indicating fra properties and time-mem effects





Polarization switching dynamics and dielectric responses

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Self-similarity of ferroelectric domain structure geometry

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Kim S. et al. //Material Letters, 2018.
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Fractal-stepwise gro models and fractional r of polarization switc

Fatuzzo E. // Physical Review, I
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INTRODUCTION & MOTIVATION

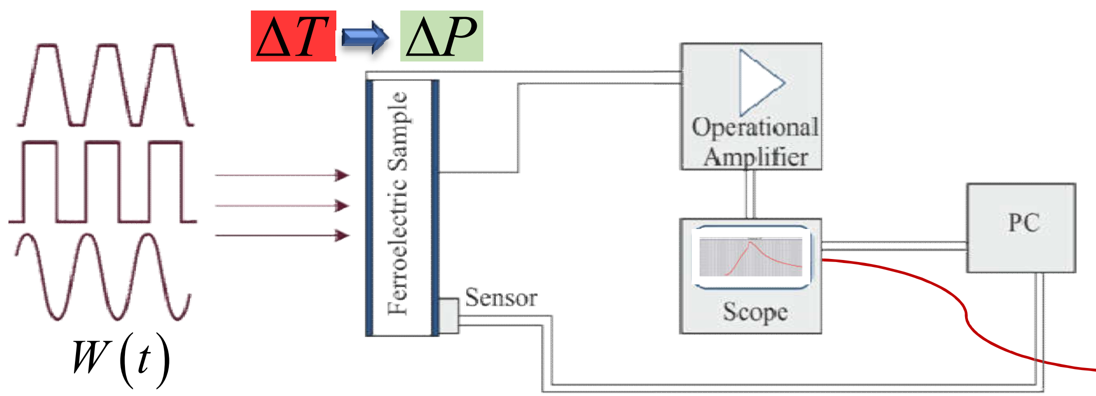
E RESEARCH FOCUS

y applications of ferroelectrics: change their polarization under external exposure

titutive pyroelectric properties of ferroelectrics: creating thermal sensors
eceivers of radiant energy to detect infrared and microwave radiations

pyroelectric effect is the change in **polarization** as a ponse to the change in **temperature**.

The pyroeffect is ially observed near Curie temperature.



A typical experimental setup for pyroelectric measurements

Experimental & theoretical stud of pyroelectric effect in ferroelec

Strukov B.A. // Physics of the Solid States, 1964
HadniA., Thomas R. // Ferroelectrics, 1972
Lal R.B., Batra A.K. // Ferroelectrics, 1993
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TrybusM. , Wos B. // Infrared Phys. Techn., 2015

Pyroelectric current: to characterize polarization in those areas of crystal which the thermal wave penetrates

Pyroelectric current: $I(t) = \frac{S}{d}\int_0^d \frac{\partial P_s}{\partial t}dx \Longrightarrow I(t) = \frac{S}{d}\int_0^d \gamma(T)\frac{\partial T(x,t)}{\partial t}dx$

S is the electrode area,
d is the sample thickness,
γ is the pyrocoefficient,
$T(x,t)$ is the temperature distribu

ectric current: response to the influence of a heat flux modulated by pulses oidal, rectangular, sinusoidal) at a defined frequency

INTRODUCTION & MOTIVATION

CONCEPT OF THE STUDY

**lopment of fractional differential models of dynamic
ponses in ferroelectrics as fractal physical systems**

lectrics possess
similar domain
ures and exhibit
memory effects

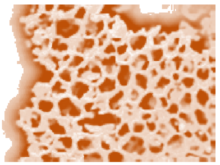
The mathematical
apparatus of
fractional
differential theory

Modelling of heat conduction
in materials characterized
by time-memory effects and
complex structures

**velopment of the time-fractional model of thermal
ses induced by modulated heat fluxes in ferroelectrics
h a focus on the application of numerical methods**

**Formalization of complex processes and phenome
based on the fractional differentiation theory**

$$\frac{d^{\beta}F}{dx^{\beta}}$$



**Self-similar properties
of materials with
nonhomogeneous structure and
multiphase composition**

$$\frac{d^{\alpha}F}{dt^{\alpha}}$$

**Time memory effect
in dynamic systems**

**FRACTIONAL CALCULUS:
MODELS, ANALITICAL & NUMERICAL METHO**

*(FODE,FPDE: Samko S.G., Oldham K., Miller A., Killbas A. A., Nahush
Deng W., Podlubny I., Petrass I., Pskhu A., Diethelm K., Meerschaert
Zhou Y., Reviznikov D.L., Meerschaert M.M., Uchaikin V., Sibatov R.T.,
V.G., Sweilam N.H., Zecova M., …)*

TIME-FRACTIONAL MODEL
OF THERMAL WAVE PROPAGATION IN FERROELECTRICS

RMALIZATION OF THE PROBLEM

$$x,\tau) = \frac{k_T t^*}{\rho c(T)}\frac{\partial^2 T(x,\tau)}{\partial x^2},\ 0<x<L,\ 0<\tau\le\theta/t^*,$$

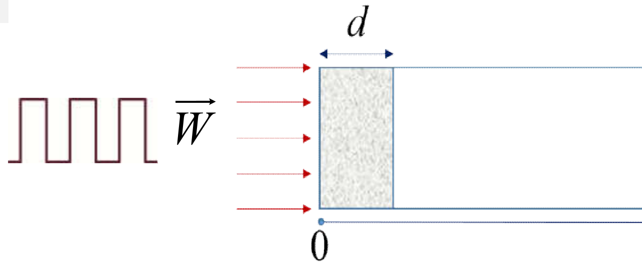
$$= T_0,\ 0\le x\le L,$$

$$\Big|_{x=0} = -W(\tau), W(\tau)=\frac{Q}{2}\Big(\mathrm{sign}\big(\sin(\omega t^*\tau)\big)+1\Big),\ 0\le\tau\le\theta/t^*,\quad T\big|_{x=L}=T_0,\ 0\le\tau\le\theta/t^*,$$

ere $T(x,\tau)$ is the temperature distribution in object in K.
the order of time fractional derivative, $0<\alpha<2$; $\tau=t/t^*$ is the dimensionless time;
the characteristic time in s; k_T is the heat conductivity coefficient in W/(m·K);
the material density in kg/m^3; $c(T)$ is the specific heat capacity in J/(kg·K);
the sample thickness (the heat problem), m;
s the ambient temperature in K;
the thermal surface power in W/m^2;
the frequency of thermal field oscillations in Hz.

INTENSIVE HEATING

Nonlinear temperature dependences of thermal physical characteris $c(T)$ and $\gamma(T)$ can be characterized by λ-shaped temperature dependen typical ferroelectrics, k_T does not have any anomaly near the temperature



The geometrical scheme of the
and heat source (the heat flu
modulated with rectangular pu

TIME-FRACTIONAL MODEL
OF THERMAL WAVE PROPAGATION IN FERROELECTRICS

NERALIZED FORMULATION

ne initial-boundary value problem in the concept of **anomalous diffusion model**

$$= d\frac{\partial^{\beta} u}{\partial x^{\beta}} + f(x,t),\ 0 < x < L,\ 0 < t \le \theta,$$

$$= u_0(x),\ 0 \le x \le L;$$

$$\left.\frac{u}{x}\right|_{x=0} + qu\big|_{x=0} - g = 0,\ \left.\frac{du}{dx}\right|_{x=L} + qu\big|_{x=L} - g = 0,\ 0 < t \le \theta,$$

ere $u(x,t)$ is the determined function;
s the diffusion coefficient;
$t)$ is the source function;
$\alpha\le2$ and $1\le\beta\le2$ are the orders
fractional derivatives with respect to space and time;
g are the model parameters.

Classification of a set of anomalous diffusion equ

At fixed order parameter β=2

- ✓ $0<\alpha<1$ – subdiffusion or delayed wanderi
- ✓ $\alpha=1$ – classical diffusion;
- ✓ $1<\alpha<2$ – superdiffusion;
- ✓ $\alpha=2$ – wave equation.

At fixed order parameter α=1

- ✓ $1<\beta<2$ – accelerated wandering;
- ✓ $\beta=1$ – classical transport equation;
- ✓ $\beta=2$ – classical diffusion process.

COMPUTATIONAL SCHEME
& IMPLEMENTATION OF NUMERICAL ALGORITHM

space-time mesh

$$= \left\{ x_i = (i-1)\Delta x,\ i = \overline{1,M},\ \Delta\tau^j = (j-1)\Delta\tau,\ j = \overline{1,N} \right\}$$

$$T_{i-1}^{j+1} + \left(v_1 + 2R_i^{j+1}\right)T_i^{j+1} - R_i^{j+1}T_{i+1}^{j+1} = -\sum_{k=2}^{j+1} v_k T_i^{j-k+2},\quad i = \overline{2, M-1},\ j = \overline{1, N-1},$$

re $R_i^{j+1} = \dfrac{k_T t^* \Gamma(2-\alpha)(\Delta\tau)^\alpha}{\rho c\left(T_i^j\right)(\Delta x)^2}$, the weight functions:

$$-\zeta(\alpha-1),$$

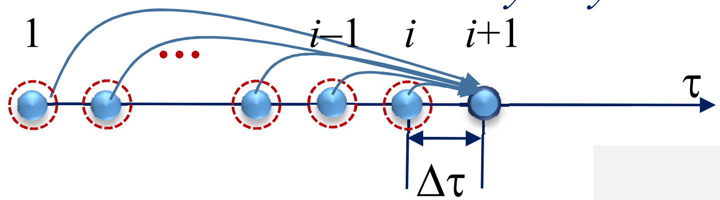
$$2^{1-\alpha} - 2 + 2\zeta(\alpha-1),$$

$$3^{1-\alpha} - 2\cdot 2^{1-\alpha} + 1 - \zeta(\alpha-1),$$

$$k^{1-\alpha} - 2\cdot(k-1)^{1-\alpha} + (k-2)^{1-\alpha},\ k = \overline{4, j},$$

$= (k-2)^{1-\alpha} - (k-1)^{1-\alpha}$, $\zeta(\cdot)$ is the Riemann zeta function.

"Full memory" dynamic system



resource intensive computations

- ✓The time-fractional derivative in Capu sense
- ✓Subdiffusion mode 0<α<1
- ✓The finite difference approximation o Caputo time fractional derivative
- ✓The modified implicit scheme
- ✓The approximation order $O\left((\Delta\tau)^2 + \right.$
- ✓The approximation of boundary condi and initial condition
- ✓ The Thomas algorithm

Approximation for the Caputo derivative

Dimitrov Yu. et al // Adv. Comp. Industr. Math., 2017

The study of the solvability, stability and convergence of the sc

Huang J. et al. // Num. Math.: Theory, Methods and Applications, 2012

Li C., Wu R., Ding H. // Commun. Appl. Ind. Math., 2015

Cao J. // Intern. J. Comp. Math., 2015

COMPUTATIONAL SCHEME
& IMPLEMENTATION OF NUMERICAL ALGORITHM

Program implementation of algorithm: Matlab software

Input
rameters:

- Thermophysical parameters and geometric characteristics of a ferroelectric crystal ($c(T)$, $\gamma(T)$, k_T, L, S, d, ρ)
- Initial temperature T_0
- Surface heat flux density Q
- Computational parameters (α, θ, t^*, mesh parameters)

he processor
part of the
program:

- Numerical solution of fractional PDE
- Computation of pyroelectric current

Output data:

- Space-time temperature distribution in the sample $T(x,t)$
- Pyroelectric response as a temporal function $I(t)$

Verification of computational res

- comparison of solutions for test problems with known analytical solutions
- comparison with the data of the numerical solution in the limiting (α=1) of solution of the integer pr
- comparison with the numerical so obtained by the finite element me using COMSOL Multiphysics sof

COMPUTATIONAL SCHEME
& IMPLEMENTATION OF NUMERICAL ALGORITHM

mple

$$\frac{\partial^\alpha U(x,t)}{\partial t^\alpha}=\frac{\partial^2 U(x,t)}{\partial x^2}+\frac{\Gamma(3+\alpha)}{2}t^2\cos(\pi x)+\pi^2 t^{2+\alpha}\cos(\pi x),\ 0<x<1,\ 0<t\le 1,$$

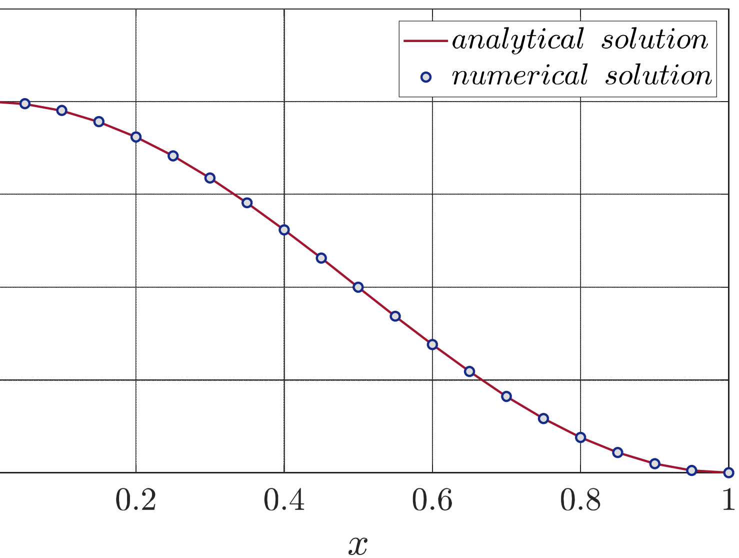
$$U(x,0)=0,\ 0\le x\le 1,$$

$$U_x(0,t)=0,\ U(1,t)=-t^{2+\alpha},\ 0\le t\le 1$$

where α=0.5 is the order of fractional temporal derivative.

$$U=v^p$$

$$\frac{\partial^\alpha U}{\partial v^\alpha}=\frac{\Gamma(p+1)}{\Gamma(p+1-\alpha)}$$



numerical solution obtained with the implicit FDM
on Caputo formula) compared to the exact solution

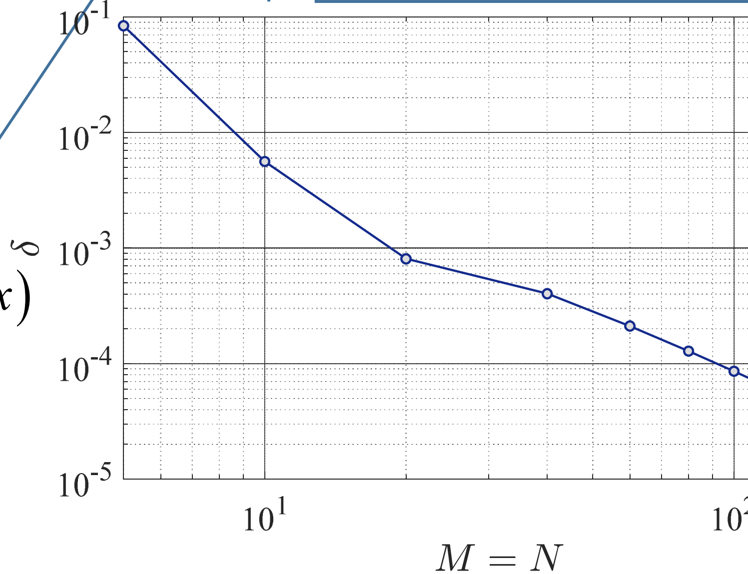
The scheme provides a converged solution and an acceptable accuracy

Exact solution:

$$U_{ex}(x,t)=t^{2+\alpha}\cos(\pi x)$$

Relative error:

$$\delta=\frac{\left\|U_{ex}-U\right\|_\infty}{\left\|U_{ex}\right\|_\infty}$$



Estimations of relative error in the log-log scale
for numerical solutions under the variation of the number of

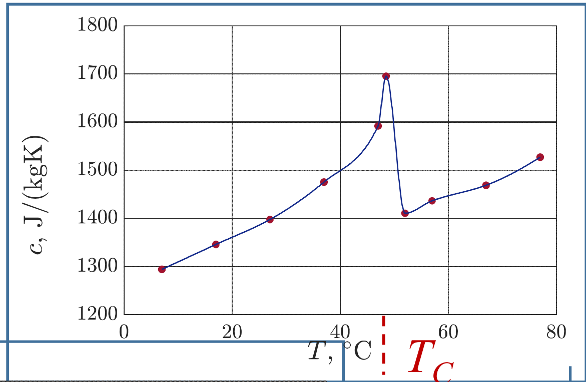
COMPUTATIONAL EXPERIMENTS

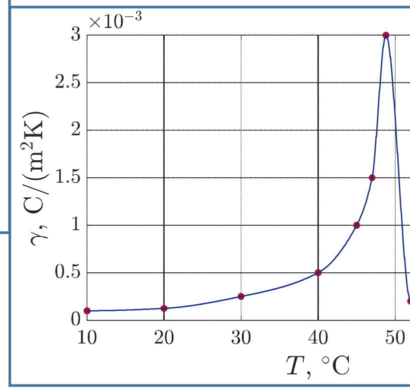
IALIZATION OF MODEL PARAMETERS

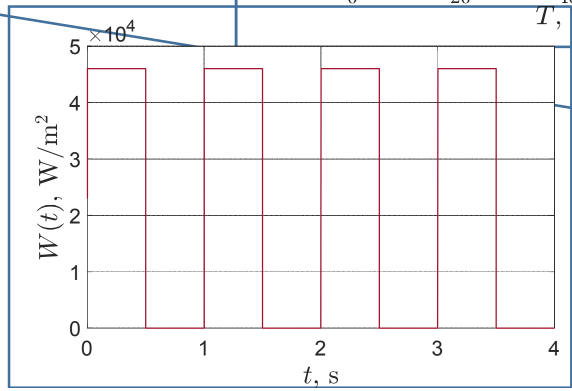
Triglycine sulphate (TGS, $(NH_2CH_2COOH)_3H_2SO_4$) is an organic water-soluble ferroelectric material having a second-order phase transition. The Curie temperature is ~49 °C.
TGS crystals are wide used as active elements in pyroelectric devices

Bogomolov A.A. et al // Ferro
1997
Strukov B.A. et al // Physics o
Solid State, 1998

heat conductivity coefficient k_T=0.8 W/(m·K),
material density ρ=1.6·10³ kg/m³;
specific heat capacity $c(T)$ and the pyroelectric coefficient $\gamma(T)$
approximations of experimental data);
surface power of source Q=1-10·10⁴ W/m²;
frequency of thermal field oscillations f=0.5-10 Hz;
linear size of object L=25 mm;
crystal thickness d=3 mm;
1 s, the simulation time – [0, 5] s.

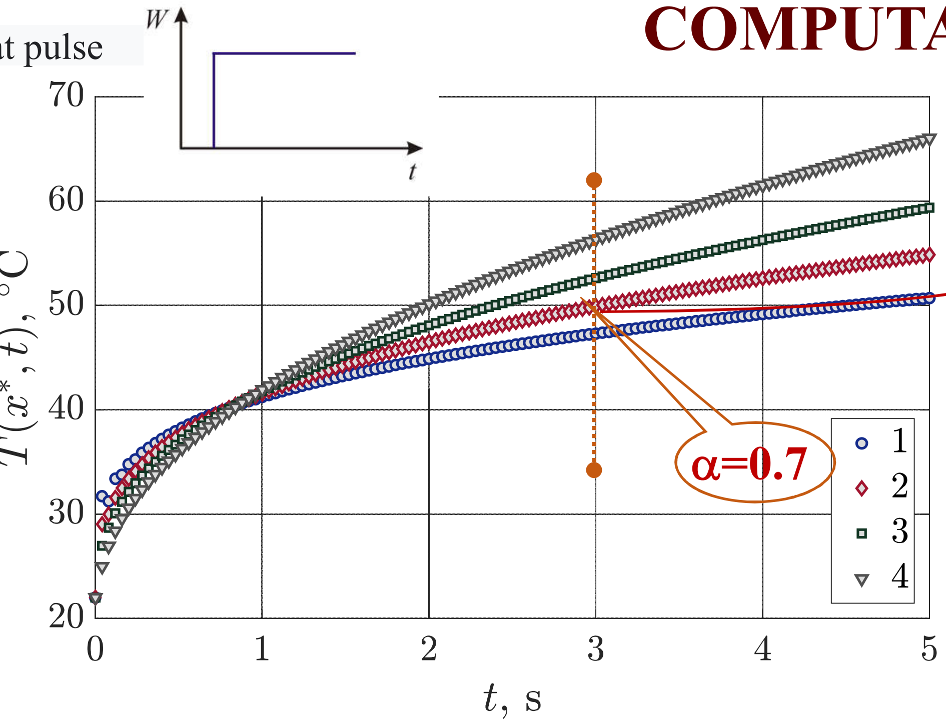






!!! The intensive heating m

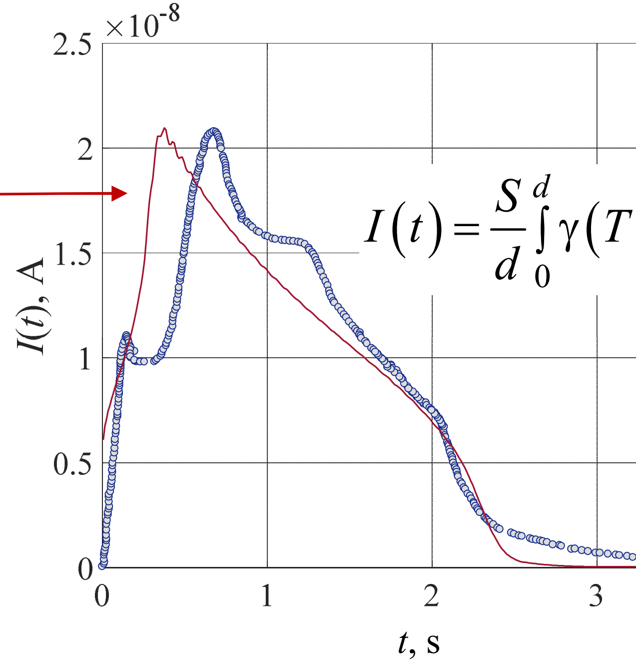
COMPUTATIONAL EXPERIMENTS



The temperature dynamics $T(x^*,t)$ for $x^*=0$
under variation of the order of fractional derivative:
1 – $\alpha_1=0.5$, 2 – $\alpha_2=0.7$, 3 – $\alpha_3=0.9$, 4 – $\alpha_4=1$) at $Q=2.3\cdot10^4$ W/m²

$T(x,t) \rightarrow I(t)$

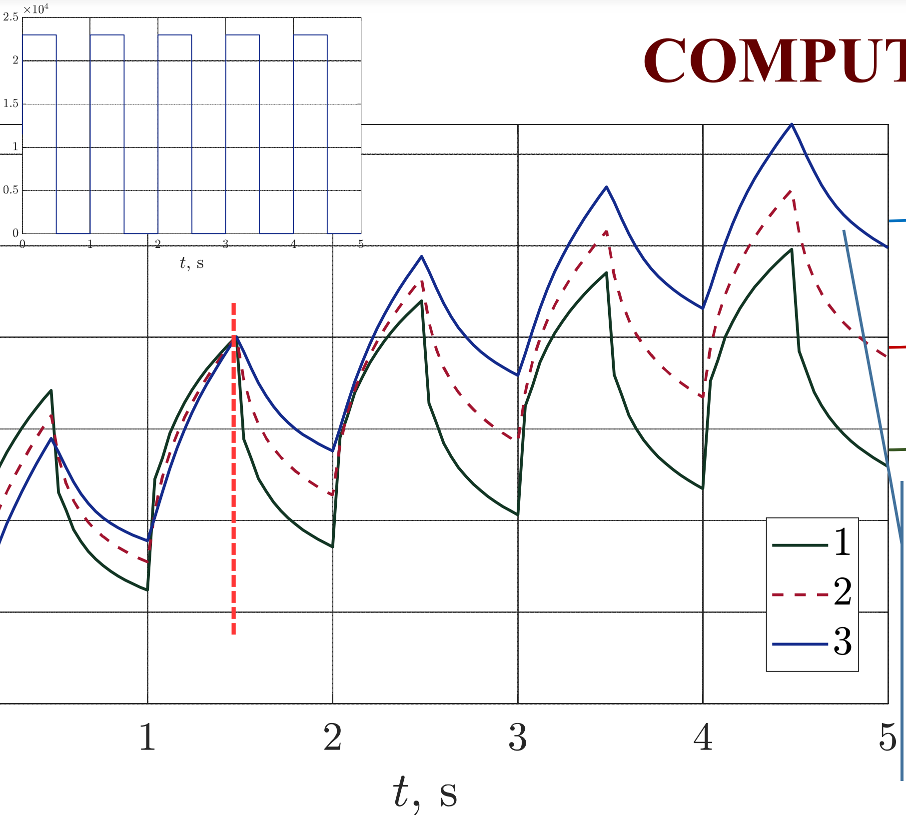
- t_C=3 s – «Curie time» is the time during which a hysteresis loop disappeared in the experiment and the crystal is heated up to Curie temperature (T_C~49°C).
- The subdiffusion mode is realized



The calculated pyroelectric current in TGS crystal (α=0
compared to the experimantal data – 1
(Kushnarev P.I., Maslovskaya A.G., Baryshnikov S.V. // Russian Physics J
Moroz L.I., Maslovskaya A.G. // Materials Science Forum, 2020)

The fractional differential model of thermal conductivity: a more adequate representation of the thermal field in the object, which is responsible for the formation of the pyroelectric response in ferroelectrics under intense heating.

COMPUTATIONAL EXPERIMENTS

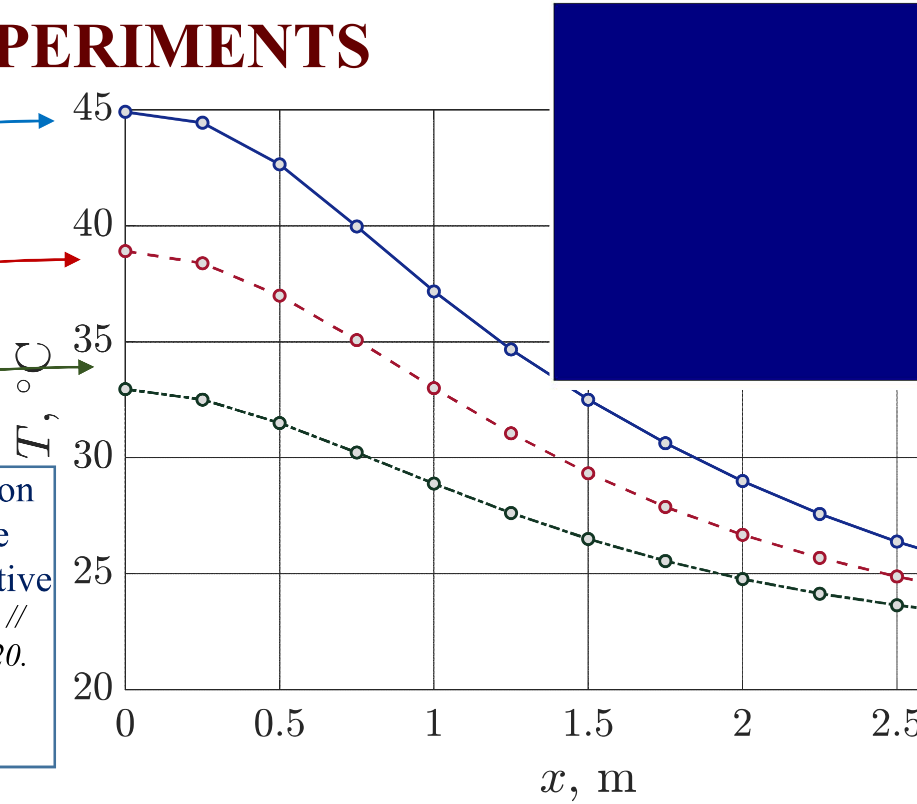


superdiffusion mode

classical diffusion

subdiffusion mode

Numerical scheme based on FD approximation of the Grünwald-Letnikov derivative
Moroz L.I., Maslovskaya A.G. // Materials Science Forum, 2020.
Kuttler C., Maslovskaya A. // Appl. Math. Modelling, 2020 .



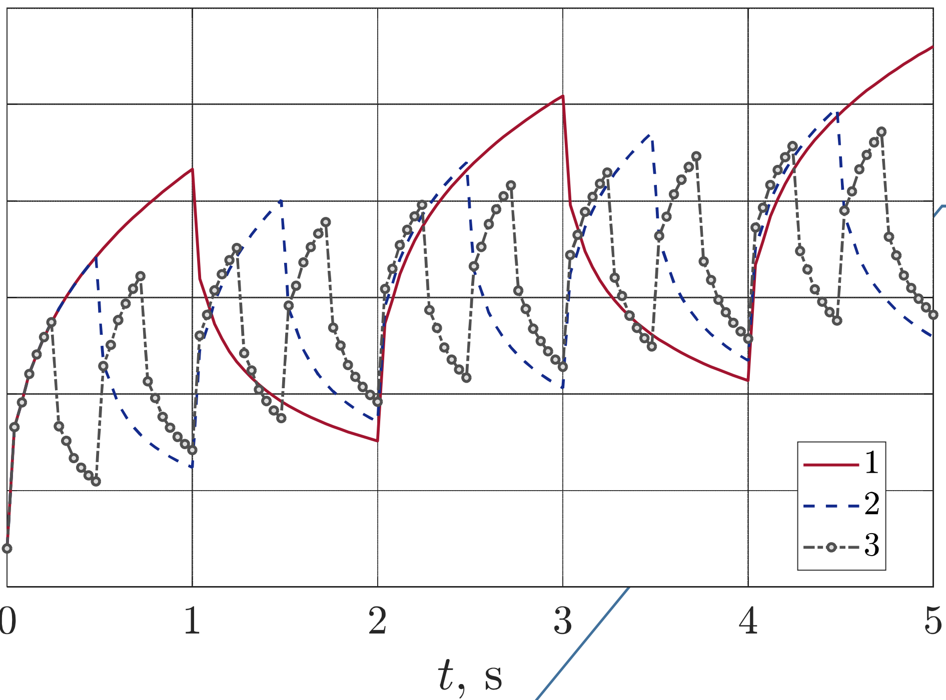
The temperature dynamics T(x,t) at x=0

The coordinate temperature distribution T(x,t) at t

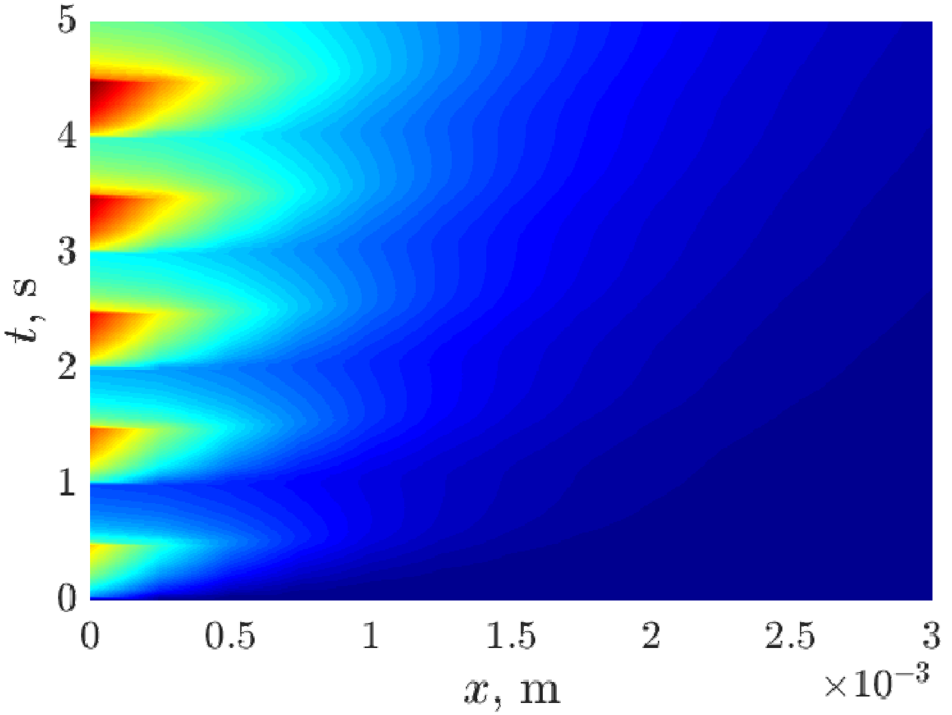
under variation of the order of time fractional derivative:
1 – α=0.7 (subdiffusion mode), 2 – α=1 (classical diffusion), 3 – α=1.25 (superdiffusion mode), $Q=2.3\cdot10^4$ *W/m*^{2}*, f=1 Hz*

e character of behavior of dynamical system changes after 1.5 seconds: more slight changes in temperature for bdiffusion mode. ➡ More than 10 degrees temperature difference on the sample surface at t=5 s.

COMPUTATIONAL EXPERIMENTS



The essential parameter for the pyroelectric dynamic method



e temperature dynamics T(x,t) at source action point x=0
er variation of the frequency of thermal field oscillations:
1 – f=0.5 Hz, 2 – f=1 Hz, 2 – f=2 Hz, Q=2.3·10⁴ W/m²

The space-time temperature distribution T(x,t) at th
of fractional derivative α=0.7, Q=2.3·10⁴ W/m², f

xperimental studies: the increased frequencies are applied (more than 5 Hz) – the exploration of polarization characteristics only for rface layers (in linear thermal mode). Computer simulations (at the application of low frequencies (less than unit)) allow one to camine the internal polarization distribution in the deep layers of ferroelectrics.

SUMMARY

- The time-fractional model as a generalization of the classical heat conductivity model has been proposed to describe thermal wave propagation in typical ferroelectrics under intense heating.
- A computational scheme for solving the time-fractional heat conductivity equation has been designed and implemented. The scheme was constructed as an analogue of the implicit scheme using the Caputo derivative for numerical solution of the nonlinear fractional heat equation.
- The considered model and computational technique underlie the hereditary modification of the model for the formation of the pyroelectric response in ferroelectrics (attributed to the method of dynamical pyroeffect).
- The simulation data indicate the subdiffusion nature of the dynamics of heat propagation and some "deceleration" – heating delay due to the specifics of time memory effects in ferroelectrics.

MANY THANKS FOR YOUR ATTENTION!

ACKNOWLEDGMENTS

RUSSIAN FOUNDATION FOR BASIC RESEARCH

RFBR

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Project “Fractional differential approach to numerical modeling of dynamic responses in complex self-similar physical systems”, No 20-31-90075