西安交通大学
XI'AN JIAOTONG UNIVERSITY

World Scientific
www.worldscientific.com

Temperature-activation mechanism of the temperature dependence of the dielectric constant of ferroelectric ceramics PZT

D. V. Kuzenko

Science & Technology Center "Reaktivelektron"
of the National Academy Science of Ukraine

Bakinskikh Komissarov Street, 83049 Donetsk, Ukraine

danil.kuzenko@gmail.com

The theoretical possibility of the temperature-activation process of the temperature dependence of the dielectric constant of samples of ferroelectric ceramics lead zirconate titanate (PZT) at temperatures below the Curie point is considered. The model takes into account the 180° motion of the domain wall, which is located in the potential well. The values of activation energies (~ 0.01, 0.1, 1 eV) were obtained from the experimental dependences of the logarithm of the dielectric constant on the reciprocal temperature. This is associated with three processes: initial vibrations of domain walls; separation of domain walls (DWs) from oxygen vacancies; the motion of DWs as a result of the motion of oxygen vacancies.

Keywords: PZT; dielectric constant; activation energy; domain walls; oxygen vacancies.

1. Introduction

One of the main parameters of ferroelectric materials is the dielectric constant, which in ferroelectrics is largely determined by the mobility of domain walls (DWs).[1] For the practical application of ferroelectric materials, it is important to know the temperature dependence of the dielectric constant, since from this dependence it is possible to determine the ranges of temperature stability of the dielectric constant.[2–6] It is known that during the operation of ferroelectrics in devices, the upper limit of permissible temperatures should not exceed half the value of the Curie temperature, since further heating of the ferroelectric sample leads to its partial depolarization. A number of works have noted the existence of a temperature below the Curie temperature, heating at which leads to a significant decrease in the piezoelectric properties.[7,8] More precisely, the boundary of the onset temperature depolarization is defined as the depolarization temperature T_d, at which an irreversible change in the piezoelectric properties of samples ceramic PZT occurs.[9,10] In these works, it was determined that heating the samples at a temperature T_d leads to the fact that after cooling the samples from this temperature to room temperature, the pattern of the diffraction spectra changes, which is determined by the rearrangement of the domain structure. This is possible only when there is an irreversible displacement of the domain walls.

In this work, the task is to determine a possible mechanism of irreversible displacement DWs upon heating a ferroelectric sample. The temperature-activation process is proposed as such a mechanism. To confirm this assumption, the dependences of the logarithm of the dielectric constant on the reciprocal temperature, obtained from the experimental temperature dependences of the dielectric constant, will be constructed, and the theoretical possibility of such a temperature-activation process through the solution of the equation motion the domain wall.

2. Materials and Methods

For the study, we used samples in the form of disks 10 mm in diameter and 1 mm thick based on ferroelectric-hard solid solutions of PZT system $((Pb_{0.95}Sr_{0.05})(Zr_xTi_{1-x})O_3)$:

- $(Pb_{0.95}Sr_{0.05})(Zr_{0.58}Ti_{0.42})O_3$ (rhombohedral symmetry),
- $(Pb_{0.95}Sr_{0.05})(Zr_{0.53}Ti_{0.47})O_3$ (morphotropic region),
- $(Pb_{0.95}Sr_{0.05})(Zr_{0.48}Ti_{0.52})O_3$ (tetragonal symmetry).

The studied PZT solid solutions are in the phase diagram of the composition (Zr/Ti) – temperature both in the region of rhombohedral (*Rh*) at $x = 0.60$ and tetragonal (*T*) at $x = 0.45$ distortions of the perovskite crystal lattice. We also have studied the solid solution from the morphotropic region ($x = 0.51$), which is characterized by the coexistence of domains of the *Rh*- and *T*-phases in the bulk of the sample.

The conventional solid-state reaction route method with high purity ingredients was employed to prepare PZT-based ceramic samples. Samples were prepared from the oxides (ZrO_2, TiO_2) and carbonates $(PbCO_3, SrCO_3)$. The doping

chemical elements were added to the mixture of PZT-based elements in the form of oxides. The resulting oxide–carbonate mixture was mixed and attrition milled for 3 h. Calcination was performed at 850°C (the first stage) for 2 h and at 1050°C (the second stage) for 2 h in alumina crucibles. The second stage was provided in PbO atmosphere. The calcined powder was ground by ball milling for 4 h. The dried powder was mixed with polyvinyl alcohol and pressed with a pressure of 1 t·cm^{-2} into discs 15 mm in diameter and about 1 mm in thickness. The sintering of ceramic samples was provided at 1250°C for 2 h in PbO atmosphere also. The density of the samples is determined by hydrostatic weighing (7.6 g·cm^{-3}) and is equal to 97% of the theoretical, which is determined by the X-ray method. The silver paste was fired on the upper and lower faces of the disc as electrodes. The silver firing was performed at 700°C for 10 min. The polarization of the ceramic samples was carried out at a temperature of 120°C in a DC electric field of 3 kV·mm^{-1} for 1 h, followed by cooling to room temperature in the field. Dielectric properties were measured using an LCR E7-8 meter at a frequency of 1 kHz with a measured field amplitude of 4 V. The piezoelectric coefficient d_{33} was measured by the Berlincourt method (quasi-static method).

The single phase of the samples was controlled by the X-ray diffractometer DRON-3 using the filtered Cu Kα emission.

The temperature dependence of the dielectric constant was determined by measuring the capacitance of a ferroelectric sample by the bridge method with a change in temperature. The sample temperature was recorded with a chromel-alumel thermocouple.

3. Equation of Motion of the Domain Wall

First of all, let us find a formula expression that allows us to draw a conclusion about the temperature-activation mechanism of the temperature dependence of the dielectric constant in the ferroelectric phase (below the Curie point). To do this, we consider the motion of the 180° domain wall in an external electric field in the presence of the following forces:

(i) pressure force due to the presence of macroscopic polarization and an alternating field: $P \cdot E \cdot e^{i\omega t} \cdot S$ (P – macroscopic polarization, $E \cdot e^{i\omega t}$ – external variable field with frequency ω, S – the area of the domain wall, which we take equal to 1 m^2);

(ii) the elastic force due to the elastic connection of the domain wall with the lattice: $c \cdot u$ (c is the stiffness of the connection between the domain wall and the lattice, u is the displacement of the domain wall);

(iii) the force of viscous resistance arising during the motion of the domain wall, which will be considered proportional to the speed of motion of the domain wall: $\eta \cdot v$ (η is the viscosity of the crystallite, v is the speed of motion of the domain wall);

(iv) resultant forces: $m \cdot a$ (m is the effective mass of the domain wall, a is the acceleration of the domain wall).

The stiffness of the bond between the domain wall and the lattice (coefficient c) and the viscosity of the crystallite (coefficient η) will be considered as average, i.e., independent of the displacement of the domain wall u, which are small in a weak measuring electric field (4 V·mm^{-1}). As a first approximation, this will simplify the problem of obtaining the equation of motion for the domain wall.

Let us graphically depict the displacement of the domain wall in the external electric field E and the forces acting on the domain wall in this case (Fig. 1).

Then the equation of motion of the domain wall will have the following form:

$$m \cdot \left(\frac{d^2 u(t)}{dt^2} \right) + c \cdot u(t) + \eta \cdot \frac{du(t)}{dt} - P \cdot E \cdot e^{i \cdot \omega \cdot t} = 0. \quad (1)$$

The general solution of this inhomogeneous differential equation is represented by the sum of the general solution of the homogeneous equation and the particular solution of the inhomogeneous equation:

$$u(t) = C_1 \cdot e^{a \cdot t} + C_2 \cdot e^{b \cdot t} + \frac{P \cdot E \cdot e^{i \cdot \omega \cdot t}}{m \cdot (\omega_0^2 - \omega^2) + i \cdot \eta \cdot \omega}, \quad (2)$$

where C_1 and C_2 are coefficients; and

$$a = \frac{-\eta - \sqrt{-4 \cdot c \cdot m + \eta^2}}{2 \cdot m}; \quad b = \frac{-\eta + \sqrt{-4 \cdot c \cdot m + \eta^2}}{2 \cdot m};$$
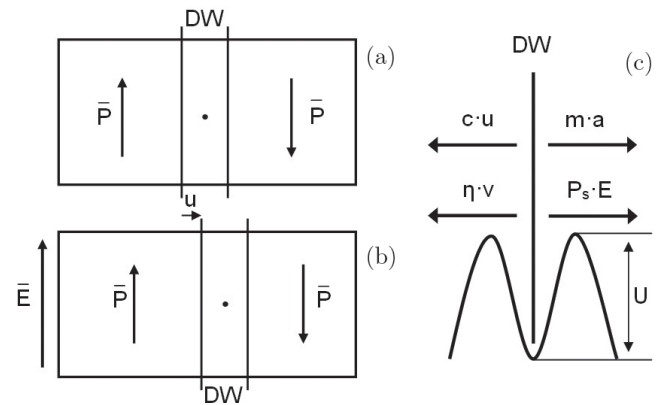
$$\omega_0^2 = \frac{c}{m}.$$

$$(3)$$

Fig. 1.   Schematically: (a) 180° domain wall (DW); (b) movement of the 180° DW in the field E, u – displacement DW; (c) forces acting on the 180° DW, which is located in the potential well, during the motion: $m \cdot a$ – resultant force; $P \cdot E$ – the force of the electric field pressure; $c \cdot u$ – elastic force; ηv – viscous resistance force; U – potential well depth.

Then the expression for polarization will have the form:

$$P = \frac{(u(t) - C_1 \cdot e^{a \cdot t} - C_2 \cdot e^{b \cdot t})(m \cdot (\omega_0^2 - \omega^2) + i \cdot \eta \cdot \omega)}{E \cdot e^{i \cdot \omega \cdot t}}. \quad (4)$$

The measuring electric field is rather weak (4 V·mm^{-1}), therefore, the dependence of polarization on electric field $P(E)$ can be considered linear[11,12]:

$$P \sim \varepsilon \cdot E. \quad (5)$$

Then the expression for the dielectric constant will have the form:

$$\varepsilon \sim \frac{(u(t) - C_1 \cdot e^{a \cdot t} - C_2 \cdot e^{b \cdot t})(m \cdot (\omega_0^2 - \omega^2) + i \cdot \eta \cdot \omega)}{E^2 \cdot e^{i \cdot \omega \cdot t}}. \quad (6)$$

The DWs move in a periodic electric field. The maximum displacement of the domain wall u_m, at which its exit from the potential well is possible, will occur at the amplitude value of the field E_m. This is achieved at time intervals that are multiples of half the period of the external alternating electric field:

$$t = \frac{T}{2} = \frac{\pi}{\omega}. \quad (7)$$

Then the expression for the dielectric constant will look like:

$$\varepsilon \sim \frac{(u_m - (C_1 \cdot e^a + C_2 \cdot e^b)) \cdot e^{\frac{\pi}{\omega}}) \cdot (m \cdot (\omega_0^2 - \omega^2) + i \cdot \eta \cdot \omega)}{E_m^2}. \quad (8)$$

It should be taken into account that the measurement of the temperature dependence of the dielectric constant occurs under the simultaneous action of an alternating electric field and thermal heating (Fig. 2).

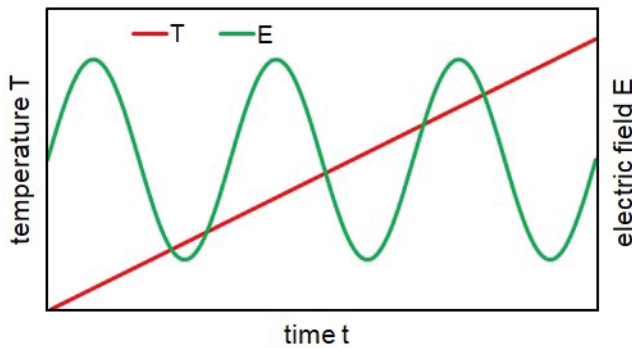Therefore, an increase in the sample temperature leads to temperature activation of the domain wall motion, which contributes to the temperature dependence of the dielectric constant. In Eq. (8), the variables that depend on the internal parameters of the ferroelectric sample (a, b, ω_0) are probably temperature dependent, but the maximum displacement of the domain wall is obviously a temperature-activated process. The process of overcoming the potential barrier is subject to an exponential dependence on the type of the Arrhenius equation. Therefore, for the temperature dependence of the maximum displacement of the domain wall, we can write:

$$u_m(T) \sim e^{-\frac{U}{k \cdot T}}, \quad (9)$$

where U is the potential barrier for a moving domain wall, k is the Boltzmann constant, and T is the temperature of the sample. Such a dependence for the velocity of the DWs is called the semi-empirical Merz law. This fact is well verified in numerous experiments and theoretical calculations for ferroelectric domain walls.[11–15]

Now, based on Eqs. (8) and (9) and the assumptions made for the temperature dependence of the dielectric constant of the ferroelectric, we can write:

$$\varepsilon(T) \sim e^{-\frac{U}{k \cdot T}}. \quad (10)$$

It should also be noted that Ref. 16 obtained an expression for the temperature dependence of the dielectric constant due to relaxation polarization (which is inherent in inhomogeneous systems, including ceramics), for temperatures below the Curie temperature:

$$\varepsilon = \varepsilon_\infty + A \cdot e^{\frac{-2B}{T}} + C \cdot e^{\frac{-B}{T}}, \quad (11)$$

where ε_∞ is electronic polarization, A, B, C are temperature-independent coefficients and T is temperature.

Thus, the presence of an exponential dependence of the dielectric constant on the reciprocal temperature (10) and (11) may indicate the temperature-activation mechanism of the temperature dependence of the dielectric constant.

4. Experimental Results

In this work, we analyzed the temperature dependences of the dielectric constant for ceramic samples of the following compositions: $(Pb_{0.95}Sr_{0.05})(Zr_{0.45}Ti_{0.55})O_3$ (tetragonal symmetry), $(Pb_{0.95}Sr_{0.05})(Zr_{0.51}Ti_{0.49})O_3$ (morphotropic region), $(Pb_{0.95}Sr_{0.05})(Zr_{0.60}Ti_{0.40})O_3$ (rhombohedral symmetry) (Fig. 3).

Constructed on their basis the dependence of the logarithm of the dielectric constant on the reciprocal temperature $\ln(\varepsilon)(1/kT)$ (Fig. 4). On these dependences, we distinguish three sections (I, II, III), which can be approximated by linear dependences:

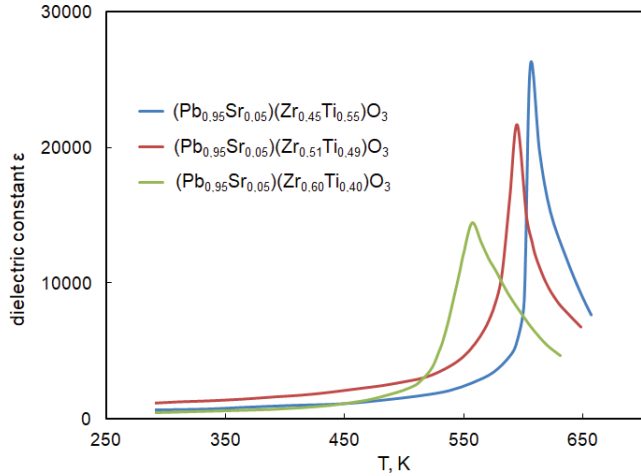$$\ln(\varepsilon) = -\frac{A}{k \cdot T} + B, \quad (12)$$

Fig. 2.   Schematically. Time dependence of the sample temperature T and the external electric field E in the measurement of the temperature dependence of the dielectric constant of a ferroelectric.

Fig. 3. Temperature dependence of the dielectric constant ε measured at 10^3 Hz with field amplitude of 4 V for ceramics specimen $(Pb_{0.95}Sr_{0.05})(Zr_xTi_{1-x})O_3$ ($x = 0.45, 0.51, 0.60$).
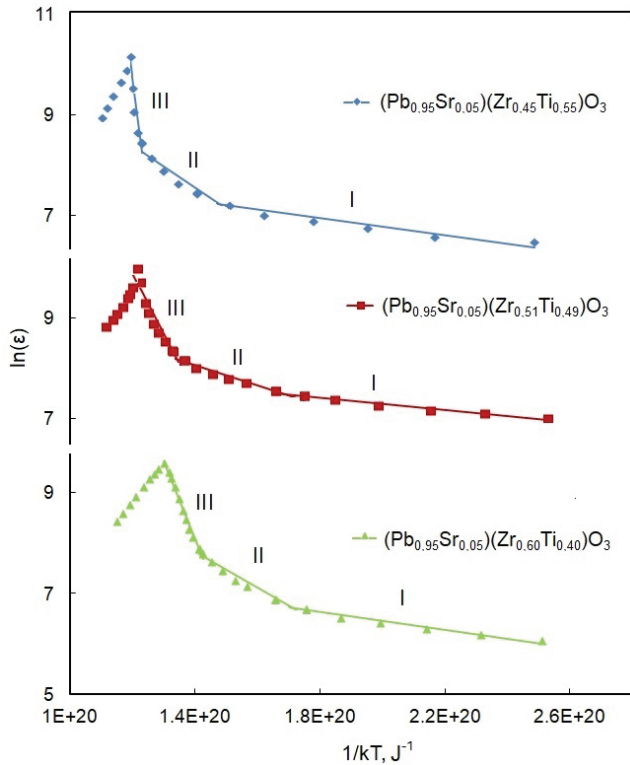

Fig. 4. Dependence $\ln(\varepsilon)$ from $1/kT$ built on the basis of temperature dependence of the dielectric constant $\varepsilon(T)$ measured at 10^3 Hz with field amplitude of 4 V for ceramics specimen $(Pb_{0.95}Sr_{0.05})(Zr_xTi_{1-x})O_3$ ($x = 0.45, 0.51, 0.60$). Plots I, II and III of the graph are approximated by a linear relationship $\ln(\varepsilon) = -A/kT + B$.

where A is a coefficient having the dimension of energy, J; B is coefficient having dimension 1; k is the Boltzmann constant; T is absolute temperature, K (Table 1).

Table 1. The coefficients A and B of the Eq. (12) for ceramics specimen $(Pb_{0.95}Sr_{0.05})(Zr_xTi_{1-x})O_3$.

Plot section		I	II	III
$x = 0.45$	A	$7.29882 \cdot 10^{-21}$	$4.68577 \cdot 10^{-20}$	$1.77318 \cdot 10^{-19}$
	B	8.21366	13.99984	30.62065
$x = 0.51$	A	$5.52247 \cdot 10^{-21}$	$2.19194 \cdot 10^{-20}$	$1.43126 \cdot 10^{-19}$
	B	8.38190	11.14051	27.19866
$x = 0.60$	A	$7.81558 \cdot 10^{-21}$	$4.04931 \cdot 10^{-20}$	$1.50391 \cdot 10^{-19}$
	B	7.99221	13.5245	29.1196

Equation (12) can be represented as follows:

$$\varepsilon = \exp(B) \cdot \exp\left(-\frac{A}{k \cdot T}\right). \tag{13}$$

Equation (13) describes the temperature-activation dependence of the dielectric constant on temperature with the activation energy A in a certain section of the dependence. Therefore, the coefficient A can be replaced by the coefficient U, which means the activation energy. The coefficient $\exp(B)$ is the value of the dielectric constant at zero activation energy $U = 0$. Let us denote it as $\varepsilon_{U=0}$. Then Eq. (13) can be represented as follows:

$$\varepsilon = \varepsilon_{U=0} \cdot \exp\left(-\frac{U}{k \cdot T}\right). \tag{14}$$

This equation has the form of the Arrhenius equation for the thermal activation process. In the discussion, we will determine the mechanism of the activation process that occurs at each temperature range.

From the obtained Eq. (14) approximating areas I, II, III for the three studied samples, the parameters of the thermal activation process were determined in three areas (Table 2) and the dependence of the activation energy on the concentration of zirconium was plotted (Fig. 5).

Table 2. The pre-exponential factors and activation energies in Eq. (14) are obtained from the dependences in Fig. 4 for samples $(Pb_{0.95}Sr_{0.05})(Zr_xTi_{1-x})O_3$.

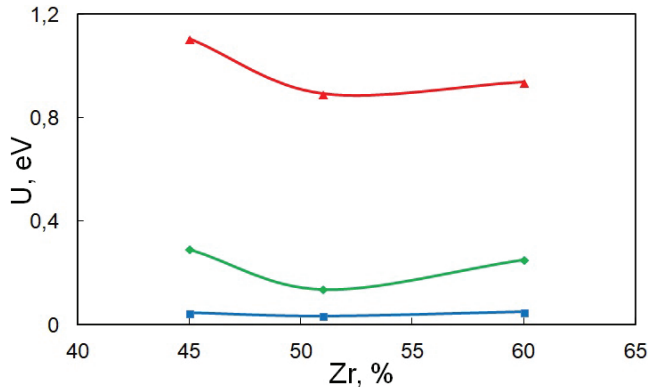| Plot section		I	II	III
$x = 0.45$	$\varepsilon_{U=0}$	3691	1202364	$1.99 \cdot 10^{+13}$
	U, eV	0.04556	0.29246	1.10673
$x = 0.51$	$\varepsilon_{U=0}$	4367	68906	$6.49 \cdot 10^{+11}$
	U, eV	0.03447	0.13681	0.89332
$x = 0.60$	$\varepsilon_{U=0}$	2958	747493	$4.43 \cdot 10^{+12}$
	U, eV	0.04878	0.25274	0.93867

Fig. 5. Dependence of energy activation U in different parts of the temperature dependence of the dielectric constant (I, II and III according to Fig. 4) on the percentage Zr for ceramic samples $(Pb_{0.95}Sr_{0.05})(Zr_xTi_{1-x})O_3$ ($x = 0.45, 0.51, 0.60$).

5. Discussion

To determine the possible mechanisms of three consecutive temperature processes with different activation energies, which are observed on the temperature dependence of the permittivity of PZT ferroelectric ceramic samples, we consider the motion of a domain wall in an external electric field in a ferroelectric containing structural defects–oxygen vacancies. In the discussions, we will discuss the literature data on this issue and connect them with the results of our study.

So, there is no doubt that much attention has been paid to the question of the influence of the motion of a domain wall on the properties of ferroelectrics. For example, the action of an alternating electric field on an interphase domain wall during a ferro–antiferroelectric phase transition was considered in Ref. 17 and an equation for the displacement of the interphase domain wall was obtained, in which the following were considered: Pressure from an expanding ferroelectric domain in an external field; the pressure of the force, which is due to the interaction of the interphase wall with stationary defects; aftereffect pressure.

An analytical expression for the motion of a 180° domain wall can also be obtained from the Landau–Khalatnikov equation in Ref. 18, which is also known as the time-dependent Landau–Ginzburg–Devonshire equation.[19–21]

One of the methods for estimating the velocity of a domain wall in a wide range of temperatures and electric fields is large-scale molecular dynamics modeling, as a result of which an inversely proportional dependence of the activation energy of motion of DWs on temperature during creep in weak fields was obtained.[22] The activation energy for the motion of DWs can also be obtained from the temperature dependence of the internal friction and the modulus of elasticity.[23] In hard undoped ceramics PZT, two relaxation peaks (R1, R2) associated with the interaction of oxygen vacancies with DWs were observed in a similar way. In addition, the

peak of the phase transition (P1) occurs at the Curie temperature. The R2 relaxation peak has already been observed with undoped PZT in Ref. 24 and cobalt-doped lead zirconate titanate in B-sites in Ref. 25. The activation energy of the R2 peak is close to the activation energy of diffusion of oxygen vacancies (0.9 eV). It is concluded that this peak is a purely relaxation mechanism controlled by the interaction between DWs and oxygen vacancies. As for the R1 peak, its activation energy is high (about 1.6 eV).[24] In Ref. 26, the activation energy was obtained for the peak R2 > 1 eV and for R1 > 1.8 eV.

The 180° domain wall motion mechanism has been explored by using the nudged elastic band method, and the effects of oxygen vacancy and in-plane strain on the domain wall motion were also investigated. And discussed the relation between the domain wall motion barriers and the 'activation field' of the phenomenological Merz law. It is found that the 'activation field' deduced from the calculated energy barrier basically agrees with the values extracted from the experimental measurement.[27] The dynamics depolarization in ferroelectric materials is described by the empirical Merz law, which gives the polarization switching time as a function of the electric field, normalized to the so-called activation field.[28] Merz law is observed in many ferroelectric systems ranging from single crystals through bulk ceramics, and thin films, to organic-ferroelectric composites.[29–32] The domain wall mobility in polycrystalline ferroelectrics–ferroelastics depends on temperature according to the Arrhenius equation, the microscopic parameters of the model including the obstacle strength and activation energy are extracted from the temperature dependence of the coercive field.[33]

Let us consider the possibility of displacing the domain wall to a new –position — overcoming the energy barrier between the two states. This means that the energy transferred to the domain wall by an external electric field and temperature heating exceeds the value of the coercive field $U > E_c$ in this place of the sample, and the sample is re-polarized locally. It should be noted that in our measurements the amplitude of the measuring electric field is 4 V·mm^{-1} (at a frequency of 1 kHz), and the process of irreversible change in the domain structure (irreversible displacement of domain walls) begins at temperatures 10–50°C below the Curie temperature.[34] The value of the coercive field measured at room temperature at a frequency of $2·10^{-2}$ Hz is up to 3 kV·mm^{-1} for ceramic samples of the composition $(Pb_{0.95}Sr_{0.05})$ $(Zr_xTi_{1-x})O_3$.[35] But with an increase in the temperature of a ferroelectric sample, its coercive force decreases linearly and near the Curie temperature takes on a value less than 50 V·mm^{-1}.[36–38]

This temperature dependence of the coercive field is explained using a micromechanical model based on the Arrhenius equation for the mobility of domain walls and is used to calculate the activation energy of motion of a domain wall in the field of short-range obstacles.[39]

Now let us dwell on the issue of estimating the activation energies of various mechanisms up to the Curie temperature in perovskites ABO_3. Numerically, the same value was obtained for the binding energy of an oxygen vacancy with a domain wall: 0.1–0.25 eV. According to estimates made for a 180° domain wall in tetragonal $PbTiO_3$ using density-functional theory, the oxygen vacancy energy decreases in the domain wall. This leads to the fact that oxygen vacancies tend to migrate to these domain walls.[40,41] In perovskite oxides, ABO_3 migration energy of oxygen vacancies is about 1 eV which obtained techniques based upon both interatomic potentials (static lattice, molecular dynamics) and quantum mechanical methods.[42]

Let us summarize the above and summarize that in our model consideration of the temperature dependence of the dielectric constant as a temperature-activation process, we obtained the Arrhenius equation for the dielectric constant. In the experimental verification of this law, we divided the dependence of the logarithm of the dielectric constant on the reciprocal temperature below the Curie temperature into three linear sections (I, II, III). Now let's define the process that takes place in each of the sections. To do this, let us schematically depict the motion of a domain wall in a potential well (Fig. 6).

When heating a ferroelectric sample, a weak measuring field ($E < 10\,V \cdot mm^{-1}$) is applied to it. This leads to vibrations of the domain walls. In section I, at temperatures up to $T \approx$ 150°C (for the studied samples PZT), the process occurring in this case has an energy of the order of $U \sim 0.01$ eV. This energy characterizes the initial oscillations of the DWs within the local potential well.

When the temperature rises above $T \approx$ 150°C, the vibration energy is of the order of $U \sim 0.1$ eV. This energy is sufficient to overcome the bond between the domain wall and pinning centers, which are oxygen vacancies in PZT samples.

Therefore, in region II, a transition of the domain wall between local minima is possible.
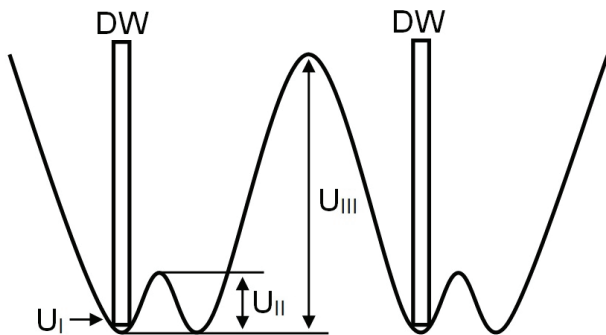

Fig. 6.   Domain wall (DW) in a potential well. U_I is the activation energy of the initial vibrations of the DW, $U_I \sim 0.01$ eV. U_{II} is the activation energy of the bond between the oxygen vacancy and DW, $U_{II} \sim 0.1$ eV. U_{III} is the activation energy of migration by DW caused by the migration of oxygen vacancies $U_{III} \sim 1$ eV.

Thermal ionization of electrons of the oxygen vacancy also begins in region II. A further increase in temperature above the temperature T_d and up to the Curie temperature T_C (Sec. 3) leads to the displacement of DWs between the main minima, since the vibration energy is of the order of $U \sim 1$ eV. As noted earlier, this energy is sufficient for the migration of oxygen vacancies, which are pinning centers for domain walls. Section 3 is also characterized by the fact that irreversible changes in the piezoelectric and dielectric properties occur here, caused by an irreversible change in the domain structure of the ferroelectric.[10]

6.   Conclusions

In this paper, we considered the possibility of describing the temperature dependence of the dielectric constant of ferroelectric ceramic samples of PZT as a temperature-activation process. As a basic position, we considered the motion of 180° domain wall, which is located in the potential well. As a result, an equation for the dependence of the dielectric constant on temperature was obtained, such as the Arrhenius equation. From the experimental dependences of the logarithm of the dielectric constant on the reciprocal temperature, the values of activation energies were obtained for three sections of the dependence, which are associated: I – with oscillations of DWs within the local potential well, $U_I \sim 0.01$ eV; II – with the transition of DWs between local minima, as a result of overcoming the connection of DWs with oxygen vacancies, $U_{II} \sim 0.1$ eV; III – with the displacement of DWs between the main minima as a result of the migration of oxygen vacancies, $U_{III} \sim 1$ eV.

References

[1] R. Xu, J. Karthik, A. R. Damodaran and L. W. Martin, Stationary domain wall contribution to enhanced ferroelectric susceptibility, *Nat. Commun.* **5**, 3120 (2014).

[2] R. Sabat, B. K. Mukherjee, W. Ren and G. M. Yang, Temperature dependence of the complete material coefficients matrix of soft and hard doped piezoelectric lead zirconate titanate ceramics, *J. Appl. Phys.* **101**, 064111 (2007).

[3] F. Li, Z. Xu, X. Wei and X. Yao, Determination of temperature dependence of piezoelectric coefficients matrix of lead zirconate titanate ceramics by quasi-static and resonance method, *J. Phys. D: Appl. Phys.* **42**, 095417 (2009).

[4] C. Miclea *et al.*, Behavior of the main properties of hard and soft type piezoceramics with temperature from 2 to 600 K, *Proc. Int. Semiconductor Conf.* (*CAS*), *October 2010* (IEEE, Romania, 2010), pp. 301–304.

[5] S. Klusacek, J. Fialka, P. Benes and Z. Havranek, An experimental study of temperature effect on material parameters of PZT ceramic ring used in knock sensors, *Proc. Seventh Int. Conf. Sensing Technology* (*ICST*), *December 2013* (IEEE, New Zealand, 2014), pp. 863–868.

[6] L. Burianova, A. Kopal and J. Nosek, Characterization of advanced piezoelectric materials in the wide temperature range, *Mater. Sci. Eng. B* **99**, 187 (2003).

[7] S. Chen, X. Dong, C. Mao and F. Cao, Thermal stability of (1-*x*)–BiScO3–*x*PbTiO3 piezoelectric ceramics for high-temperature sensor applications, *J. Am. Ceram. Soc.* **89**(10), 3270 (2006).

[8]G. A. Rossetti, Jr, A. G. Khachaturyan, G. Akcay and Y. Ni, Ferroelectric solid solutions with morphotropic boundaries: Vanishing polarization anisotropy, adaptive, polar glass, and two-phase states, *J. Appl. Phys.* **103**, 114113 (2008).

[9]D. V. Kuzenko, V. M. Ishchuk, A. I. Bazhin and N. A. Spiridonov, Relaxation processes in lead zirconate-titanate based piezoelectric ceramics. 2. Influence of thermal treatment, *Funct. Mater.* **18**(1), 66 (2011).

[10]D. V. Kuzenko, Critical temperature below the Curie temperature of ferroelectric ceramics PZT, *J. Adv. Dielect.* **11**, 2150006 (2021).

[11]V. M. Ishchuk and D. V. Kuzenko, *F*-center mechanism of long-term relaxation in lead zirconate-titanate-based piezoelectric ceramics 1. After-heating relaxation, *J. Adv. Dielect.* **5**(4), 1550036 (2015).

[12]A. N. Morozovska, E. A. Eliseev, D. Remiens and C. Soyer, Theoretical description of ferroelectric and pyroelectric hystereses in the disordered ferroelectric-semiconductor films, *J. Appl. Phys.* **100**, 014109 (2006).

[13]W. J. Merz, Domain formation and domain wall motions in ferroelectric $BaTiO_3$ single crystals, *Phys. Rev.* **95**, 690 (1954).

[14]V. Boddu, F. Endres and P. Steinmann, Molecular dynamics study of ferroelectric domain nucleation and domain switching dynamics, *Sci. Rep.* **7**, 806 (2017).

[15]R. C. Miller and G. Weinreich, Mechanism for the sidewise motion of 180° domain walls in barium titanate, *Phys. Rev.* **117**, 1460 (1960).

[16]Yu. M. Poplavko, *Физика Диэлектриков* (Киев 1972).

[17]V. M. Ishchuk, Peculiarities of ferro-antiferroelectric phase transition. 5. Relaxation dynamics of interphase domain walls, *Ferroelectrics* **234**(1–4), 151 (1999).

[18]A. S. Starkov and I. A. Starkov, Domain wall motion in the electric field of a piezoforce microscope probe: The effect of curvature and geometry of the domain wall, *Ferroelectrics* **539**, 28 (2019).

[19]Y. Kim *et al.*, Non-Kolmogorov–Avrami–Ishibashi switching dynamics in nanoscale ferroelectric capacitors, *Nano Lett.* **10**(4), 1266 (2010).

[20]A. Starkov and I. Starkov, Domain wall motion for slowly varying electric field, *Ferroelectrics* **442**(1), 1 (2013).

[21]Q. Meng *et al.*, Velocity of domain-wall motion during polarization reversal in ferroelectric thin films: Beyond Merz's Law, *Phys Rev B* **91**, 054104 (2015).

[22]S. Liu, I. Grinberg and A. M. Rappe, Intrinsic ferroelectric switching from first principles, *Nature* **534**, 360 (2016).

[23]H. Frayssignes *et al.*, Internal friction in hard and soft PZT-based ceramics, *J. Eur. Ceram. Soc.* **24**, 2989 (2004).

[24]E. M. Bourim *et al.*, Elastic modulus and mechanical loss associated with phase transitions and domain walls motions in PZT based ceramics. *J. Phys. IV* **6**, 633 (1996).

[25]C. Wang, Q. F. Fang and Z. G. Zhu, Internal friction study of $Pb(Zr,Ti)O_3$ ceramics with various Zr/Ti ratios and dopants, *J. Phys. D. Appl. Phys.* **35**, 1545 (2002).

[26]E. M. Bourim and H. Tanaka, Domain wall motion effect on the anelastic behavior in lead zirconate titanate piezoelectric ceramics, *J. Appl. Phys.* **91**, 6662 (2002).

[27]L. Xiaoyu *et al.*, Domain wall motion in perovskite ferroelectrics studied by nudged elastic band method, *J. Phys. Chem. C* **122**, 3091 (2018).

[28]Z. Dong *et al.*, Depolarization of multidomain ferroelectric materials, *Nat. Commun.* **10**, 2547 (2019).

[29]S. Zhukov *et al.*, Dynamics of polarization reversal in virgin and fatigued ferroelectric ceramics by inhomogeneous field mechanism, *Phys. Rev. B* **82**, 014109 (2010).

[30]J. Y. Jo *et al.*, Nonlinear dynamics of domain-wall propagation in epitaxial ferroelectric thin films, *Phys. Rev. Lett.* **102**, 045701 (2009).

[31]A. Gruverman, D. Wu and J. F. Scott, Piezoresponse force microscopy studies of switching behavior of ferroelectric capacitors on a 100-ns time scale, *Phys. Rev. Lett.* **100**, 097601 (2008).

[32]A. Nautiyal *et al.*, Polarization switching properties of spray deposited $CsNO_3$: PVA composite films, *Appl. Phys. A* **99**, 941 (2010).

[33]A. Yu. Belov and W. S. Kreher, Simulation of microstructure evolution in polycrystalline ferroelectrics–ferroelastics, *Acta Mater.* **54** 3463 (2006).

[34]D. Phelan *et al.*, Role of random electric fields in relaxors, *PNAS* **111**(5), 1754 (2014).

[35]D. V. Kuzenko, V. M. Ishchuk, A. I. Bazhin and N. A. Spiridonov, Long-time after effects and relaxation in piezoelectric ceramics, *Ferroelectrics* **474**, 156 (2015).

[36]V. M. Ishchuk and D. V. Kuzenko, F-centers mechanism of long-term relaxation in lead zirconate-titanate based piezoelectric ceramics. 2. After-field relaxation, *J. Adv. Dielect.* **6**(3), 1650019 (2016).

[37]M. Vopsaroiu *et al.*, Polarization dynamics and non-equilibrium switching processes in ferroelectrics, *IEEE Trans. Ultrason. Ferroelectr. Freq. Control* **58**(9), 1867 (2011).

[38]A. Yu. Belov, W. S. Kreher and M. Nicolai, The evaluation of activation parameters for ferroelectric switching in soft PZT ceramics, *Ferroelectrics* **391**(1), 42 (2009).

[39]R. Indergand, A. Vidyasagar, N. Nadkarni and D. M. Kochmann, A phase-field approach to studying the temperature-dependent ferroelectric response of bulk polycrystalline PZT, *J. Mech. Phys. Sol.* **144**, 104098 (2020).

[40]A. Chen, Y. Zhi and L. E. Cross, Oxygen-vacancy-related low-frequency dielectric relaxation and electrical conduction, *Phys. Rev. B* **62**, 228 (2000).

[41]L. He and D. Vanderbilt, First-principles study of oxygen-vacancy pinning of domain walls in $PbTiO_3$, *Phys. Rev. B* **68**, 134103 (2003).

[42]M. S. J. Islam, Ionic transport in ABO_3 perovskite oxides: A computer modelling tour, *J. Mater. Chem.* **10**, 1027 (2000).