Chapter 9

The relation of bulk elasticity with the parameters of the influence in magnet –containing metals, dielectrics and ferroelectrics

9.1. Regularities of the first-order structural phase transition in MnF_2

The magnetic and magnetoelastic properties of magnetodielectrics are vast ranges of investigations in the solid-state physics. While analyzing results of experimental investigations near the region of phase transition, we pay attention to the common nature of the magnetic states in the vicinity of the structural phase transitions. The influence of magnetic field H on the properties of magnetostriction has been analyzed for the simplest two-component representatives of magnetodielectrics that are MnF_2 single crystals being uniaxial, low-compressible and prepared by high-temperature annealing and based on transition metals with the declared first-order phase transition at 0^oK [188].

The magnetic properties of the substances with the jump of the magnetization observed at the magnetic field other than zero have been widely investigated. It should be added that for this system, the first-order structural phase transition develops with the positive dynamics of dT_p/dH and dT_p/dP changes. For the distinguished phases, the magnetization is different in the absolute value and direction.

The first-order phase transitions in the external magnetic field are discussed in [1] with mentioning the jump of the properties where the values of the field H are critical and the specific magnetization on the phase states is of different value and of different dynamics of the changes of each phase.

MnF_2 is a popular magnetodielectric for the experimentalists. It has a rutile-type crystal structure (the space group D_{4h}^{14}). The tetragonal unit cell with the parameters a=4.87 A and c=3.30 A [189] contains two Mn^{2+} ions. The manganese ion has the half-filled d-shells, five uncompensated electrons, i.e. the total spin of the ion is 5/2. The decompensation magnetic moment is of purely spin origin. For T-67 K [190], the phase transition and the jump of the magnetic susceptibility are noted [191].

The elastic constants of the crystal have been estimated [192], the thermal properties are investigated in [193], the magnetic ordering on the temperature dependence of the heat capacity have been stated [194], the coefficient of the

thermal expansion is determined as $\frac{1}{T_N}\frac{dT_N}{dP} = 4.5 \cdot 10^{-2}\ cm^2/erg$ [195], as well as the state of the additional compression (the volume change) of the crystal along the axis of the symmetry has been revealed. The magnetoelastic properties and their regular change during the PT under pressure have been distinguished [196].

In [197], the temperature dependence of the magnetic susceptibility in low fields is studied. At temperatures higher than the critical one associated with PT, the magnetic susceptibility is isotopic and obeying the Curie-Weiss law. At low temperatures, $X=10^{-3}$ units CL-SM is normal to the axis of symmetry and does not depend on the temperature. In the field aligned with the axis of symmetry, the susceptibility drops to zero with T decrease [198].

The demonstrative are studies of magnetic properties at low temperatures and high magnetic fields [199]. On the dependence of the magnetization, there is a jump of the properties typical of the first-order phase transition (Fig. 9.1b). The properties are shown at the distinguished point for T=4.2 K and for varied magnetic field orientation. Thus, in the field parallel to the axis of symmetry, there is a magnetization jump for H of 10^5Oe. The investigations show that $H_e \sim 1.1 \cdot 10^6\ Oe$, $H_a \sim 8.6 \cdot 10^3\ Oe$, i.e. there is a correspondence between exchange and anisotropic fields [200]. The rare results do not enable us to judge the first-order phase transition by the character of the magnetization curves.

Let us now to consider the experiments with ultrasound adsorption in the region of PT [201] and to analyze the magnetic properties by using the phase diagram of MnF_2 (Fig. 9.1a). On Fig. 9.1b, the considered $T_p(H)$ dependence is a field-temperature curve with the critical points PP_x and the temperature parameter evolution corresponding to the regularity of the first-order phase transition for T_{cm}(T_x=0 K, H_x~90 kOe) and of the phase transition changes with the plus sign. The anomalies of the ultrasound absorption observed near this dependence of PT can be related to the critical region separating phase states.

It has been detected that for H=93 kOe directed along the axis of the symmetry, the magnetostriction has demonstrated a jump of the crystal size [190], a change of the length in high H that is also typical of the first-order structural phase transition. These studies help in the estimation of the magnetoelastic constants for MnF_2: $A_0=8.6 \cdot 10^{-13}$cm^2/erg, $A_1=2.1 \cdot 10^{-13}$cm^2/erg, $A_2=1.07 \cdot 10^{-13}$cm^2/erg.

Investigations of the region where the structural phase transition is formed impose demands upon experimental methods. Broad temperature range is implied starting from 4.2 K and lower. For MnF_2, the magnetic fields are of 10^5-10^6 Oe with high homogeneity of the fields, high accuracy of the

orientation of the external field with respect to crystallographic axes as well as the detailed study of the field-temperature dependence of the resonance absorption in the vicinity of PT.

The explicit jumps of the magnetization properties (Fig. 9.1c) let us to assume that in MnF_2, the first-order structural phase transition restricts the phase states, changes the volume and the symmetry of each phase. This results in differences in the magnetization as well as in changes of the direction of magnetic non-compensation along crystallographic axes (different specific magnetizations) of neighbor phases relatively to changes of the crystal symmetry.

The magnetization jumps are natural factors of the formation of the structural phase transition.

The considered investigations make us to conclude that the phenomenon of jump-like magnetization change is a typical sign of physical processes of T, H effect under which the PT is formed through the mechanisms of elasticity, magnetic elasticity and important elastic and magnetoelastic anisotropy. The jump-like magnetization change is a sudden change of the properties in a narrow range of fields H~670 Oe. On the background of repeated jumps, there is a region of angles of the field deviation with respect to crystal symmetry, to within $\psi \sim 30'$. This is shown by magnetization properties on the oscillogramm of Fig. 9.1b'.

The studied phase states differ by the degree of magnetization, first of all. The experimentally observed changes are characterized by different intensity of magnetic non-compensation and magnetization jump in MnF_2 for H_c=92 kOe makes 100 units of CG-SM. The inhomogeneity of the phases in the course of PT realization is revealed by the critical range of fields and angles. While considering and drawing analogies with formation of the first-order structural phase transition in $CuCl_2 \cdot 2H_2O$ and MnF_2, let us now to analyze the field-frequency resonance absorption branch [202]. For MnF_2, the field-frequency dependence was realized in the temperature range of 4.2 K with high-accurate magnetic field orientation along the tetragonal crystal axis for frequencies of 3.5-16.5 cm^{-1}. For two single crystals of highly accurate orientation, the resonance absorption decreases the intensity of the second absorption line to the level of resolution near the PT. At low angles of deviation, the absorption was restored. For MnF_2, the fields of Pt region correspond to H~0.1+0.005T. The investigated samples were in the form of plates, L=3.5 mm and h=0.07-1.5 mm [188].

Form the above results, it can be concluded, that the regularity of the formation of the jump of the properties under the first-order structural phase transition is common of magnetodielectrics having different composition and compressibility factors. The results obtained for MnF_2 are observed for another systems of different compositions still their properties are varied in a similar

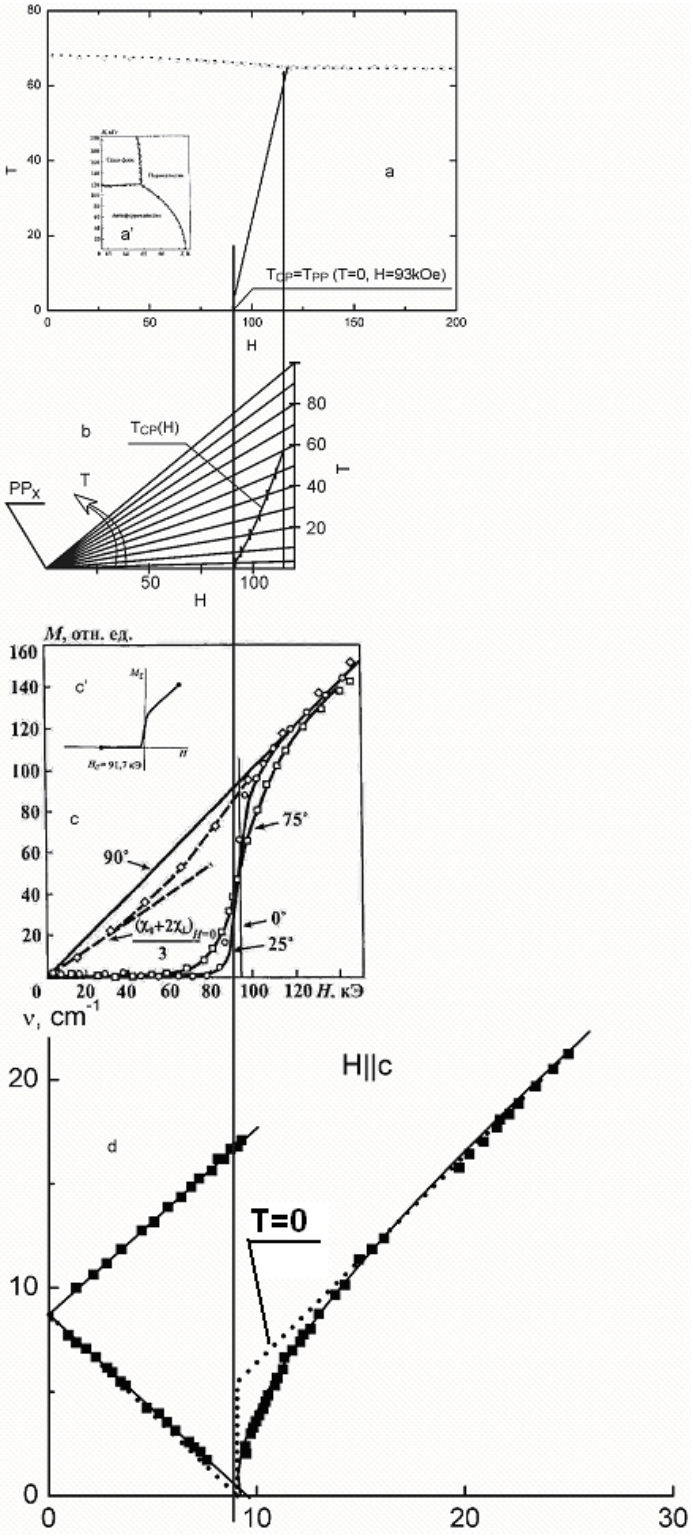

Figure 9.1. (a, a') Magnetic phase diagram MnF_2 in the field parallel to (001) axis. (b) Temperature and field dependence of a structural phase transition of the first order with separated critical point PP_x and T_{pp} (T_x=0, H_x~93 kOe). (c, c') The jump of magnetization of MnF_2 at varied orientation of magnetic field with respect to (001) axis at T=4.2 K. (d) Frequency and field dependence of resonance absorption of MnF_2 in the field parallel to (001) axis at T=4.2 K [202].

way [188]. The magnetic non-compensation is maximal along the principal crystallographic axis c, which is relatively small and for the transition to be realized at the point of 0 k, high magnetic field H=90 kOe is necessary (see the dotted line on Fig. 9.1d).

The crystal and magnetic structure of MnF_2 as well as the elastic deformation of the crystal lattice in high magnetic fields are related to the magnetostriction through the mechanisms of magnetoelastic influences under magnetization of the crystal and this is the causal basis for the changes of the properties, which are generalized by regularity of the bulk elasticity effect.

Another confirmation of the results on determination of the region of the structural phase transition in MnF_2 is work [199] where the magnetic susceptibility was studied using the samples of different shape. The specific run of the magnetization curves in the region of the jump of the properties for H~92 kOe and T=4.2 K is noted in the initial section. In low fields, the magnetization is low. Then, there follows a jump and a considerable change of the properties (Fig. 9.1c). Here we remark the analogies of the results. A correspondence to the magnetization jump in $CuCl_2 \cdot 2H_2O$ is present in lower fields and another temperatures (see [7]).

It follows that as dT/dH, $T_p(H)$ regularity is of positive sign and in the both cases we have the first-order phase transition. Thus, we get $T_p(T_x=0, H_x=90$ kOe) for MnF_2 and $T_k(T=0, H_x=5.5$ kOe) for $CuCl_2 \cdot 2H_2O$. It is also seen that for those single crystals the compared coefficients of compressibility differ by an order of magnitude, but there are regularities of H change in higher fields and PT dynamics corresponds to the “cooling-heating” effect that is an increase of H resulting in T increase at $T_p(H)$, and on the contrary, the reduction of H decreases T. Note that single crystal orientation and the sample shape are in direct correlation with the physical process of the structure change at the expense of elasticity anisotropy restricting the region of PT formation to 0.4kOe for a cylinder and 0.9 kOe for a disc.

Form the analysis of the field-temperature dependences for MnF_2 (Fig. 9.1c) and approximation thereof to 0 k we can distinguish the frequency – independent region which has not been determined in the low-temperature range for 4.2 K. With the highly accurate orientation of the magnetic field, the same was observed and characterized by the position of the structural phase transition in $CuCl_2 \cdot 2H_2O$ single crystal (Fig. 7.8). Thus, it can be concluded that from the results obtained for alloys based on 3d and 4d tetragonal structure elements, the role of mechanisms of elastically deforming stresses and the anisotropy of elasticity is the determining one with respect to the physical properties of the volume change. The result confirming the analogies with the regular change of the properties on Fig. 9.1a,b,c,d for MnF_2 and Fig. 7.8a,b,c for $CuCl_2 \cdot 2H_2O$ is the identity of the field-temperature dependences for the first-order PT, T_p with the distinguished critical point PP_x and of the field –

frequency dependence with the change at 0 K shown by the dotted line as well as with the region that fixes the positions of PT and phase states.

While separating the changes of the magnetic properties under magnetoelastic effect in the superconducting phase state and drawing analogies with the alternating mechanism of hydrostatic pressure effect on the structure inhomogeneity and PT character, it is possible to relate the regions of the superconducting phase state and magnetism with the processes of the changes of the volume and the symmetry.

The analysis of the results of the changes of the field dependences is concentrated on magnetoelastic, magnetic, electronic, structural interactions connected with the structure rearrangement at the expense of the stresses created by the magnetic field through the mechanisms of magnetic elasticity, which affect both the structural changes and the processes of formation of the region of the first- and second-order structural PT that are recorded by the resonance methods in high magnetic fields and under the hydrostatic pressure. Showing the experimental results for real physical processes, we try to attract the attention of researchers stating that theoretical models are needed taking into account the energies of elastically deforming stresses and applied to a practical case. The analysis and the methods used to ground the analogies in the study of magnetodielectrics and superconductors enable us to generalize and to connect the regularities of magnetostriction and structural changes occurring during the formation of the first-order structural phase transition. As a consequence, the changes of magnetization and magnetostriction are in accordance with the general regularities of magnetoelasticity that is a part of the total bulk elasticity.

9.2. The laws of elasticity in the mechanisms of T-H-P effect on the formation of the structural phase transitions and properties of metals

As far back as the 20-30ies of the last century, the origination and the development of the methods employing high magnetic fields and low temperatures stimulated the investigation of the electronic properties of metals. The changes of the electrical resistance in magnetic fields were studied first in bismuth. Later, this phenomenon was found in all the metals and explained by the electron conduction theory by J. Thomson [204]. The theory showed that the change of the resistance was proportional to the square law. However, in fields of about 300 kOe [205], the regularity was found violated and substituted for stable linear changes. More than 30 metals of high purity were investigated and the low-field conductance followed the square law of the changes in every metal. In high magnetic fields, the changes were linear (Fig. 9.2). For all the investigated metals, there was one more interesting

phenomenon: a chemical additive changed the position of the square dependence without changes of the linear behavior. This meant that whereas the crystallographic lattice of the metal was distorted by a physical or chemical factor, the linear law of the changes was connected immediately with the high magnetic field effect on the elastic stresses thorough magnetic elasticity resulting also in deformation of the structure. This pointed to a close relation between the state of the metal crystal lattice and the magnetic field effect.

The results of experimental investigations of physical and chemical imperfections of crystals show the phenomena due to resistance growth to be similar. The introduction of such parameter as the temperature revealed the similar changes as well [206], but with some exceptions. On Fig. 9.3, there are typical curves of the resistivity changes for copper studied at 86 K liquid hydrogen temperature as well as 63 K and 20 K of liquid hydrogen. They consist of square sections in low fields and linear ones in high fields.

With this result, some more regularity can be distinguished. In view of the influence of two thermodynamic parameters, it can be concluded that the above dependence is a consequence of two mechanisms resulting in crystallographic changes. At the beginning, the thermoelastic expansion and themagnetoelastic compression form the square dependence of the changes.

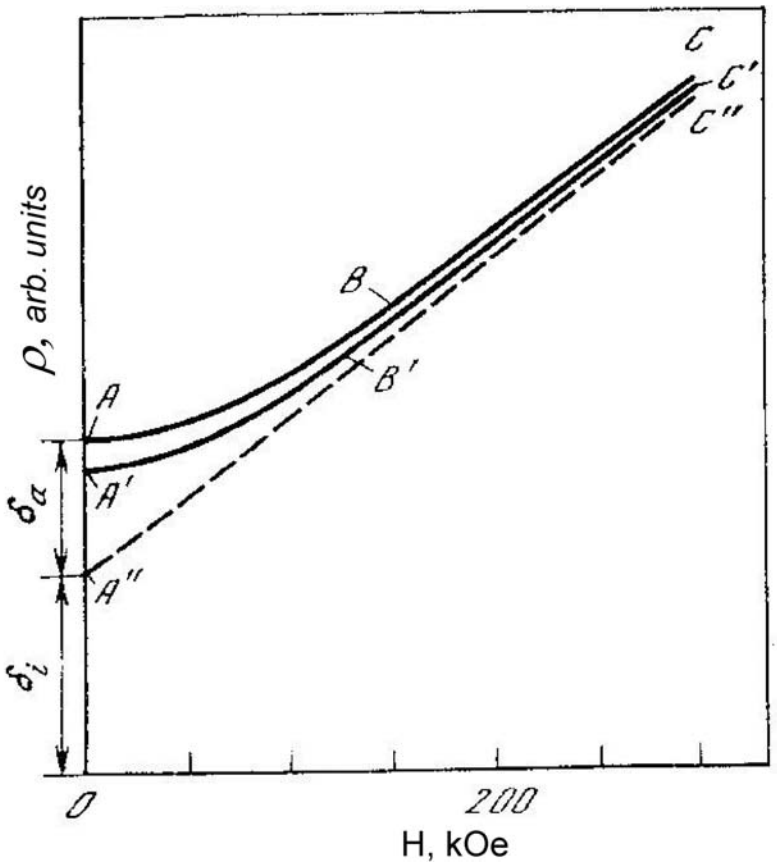

Figure 9.2. The magnetoresistivity in pure metals [205].

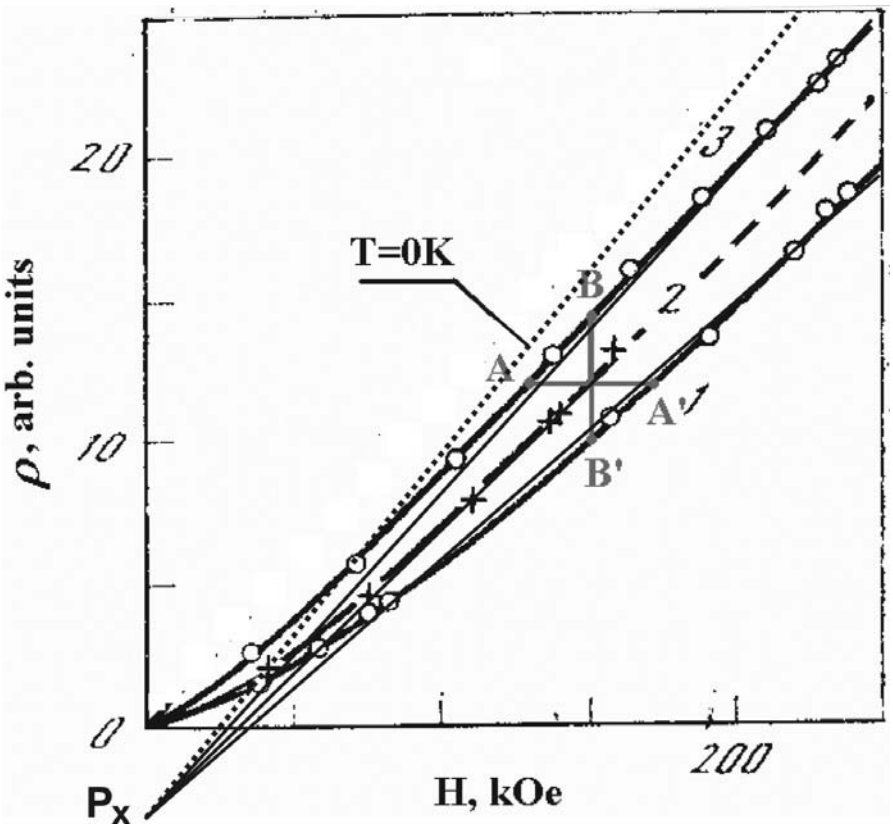

Figure 9.3. The magnetoresistivity in copper at fixed temperatures: T_1=86 K, T_2=63 K, T_3=20 K [206].

Then, a sign change follows with the preference given to the magnetoelastic effect resulting in the linear dependence due to crystallographic changes through the mechanisms of elastic stresses. The next fact of T and H effect on the physical process allows us to show the regularities of the changes (dotted line, by approximation) of the resistivity at 0K and those of cooling-heating effect from magnetic field H. The triangles ABC show how the temperature reduction increases the parameter of resistivity of fixed H (Fig. 9.3). The consequent decrease of H brings the system to the “heating” effect that is to the initial resistivity value. There is an opposite “cooling” effect which is compensated by the properties and the temperature effect with H rising. This means that the thermoelastic expansion effect brings the structure back to the initial state due to the counteraction to the magnetic compression.

Such presentation differs from the proofs suggested by Sommerfeld [206] and other theoreticians being sure that the magnetic field influences the trajectory of conduction electrons thus resulting in the changes of the properties.

Here, it is worth to mention the definitions by P.L.Kapitsa [207]. He stated that the resemblance between the resistivity growth due to crystal lattice imperfections and due to the changes of the magnetic field means that

theoretical presentations should be based on direct disturbance of the lattice structure by magnetic field. This opinion is also supported by the fact that in a number of diamagnetic substances, the magnetic field effect at low temperatures becomes apparent in magnetostriction properties. There, it was also assumed that the magnetostriction effect is a direct factor determining the relationship and the interaction of atoms in the lattice.

The lattice distortions by the deformation can be distinguished experimentally by X-ray diffraction method. However, X-rays show change of the relative intensity of the reflections of different order. The observation of the changes is difficult under short-term strong magnetic fields. Such results could not be convincingly explained from the position of the structural changes and T-H effect for about 30 years. From the position of the classical theory of the electronic properties of metals, the energy spectrum of conduction electrons does not practically differ from that of free electrons. According to this model, the energy of charge carrier is a square function of the pulse, the same as with free electrons, however their masses differ very much.

The action of crystal-lattice periodic potential on the conduction electrons is accounted for by the effective mass thereof that differs much from the mass of the electron. As a consequence, it should be taken into account that the atoms of magnet-containing sites (molecules) form the crystal lattice while the electron orbits of neighbor (valence or free) electrons intersect each other. This means that the electrons of onsite make bonds (intersect) with another site and vice versa. This implies that the energy of electrostatic interactions of the electrons will correspond to and form magnetic non-compensation or compensation with respect to the spin orientation.

While analyzing the resistivity change under H influence, the author of [207] assumed that the strong magnetic field induced changes of the crystal structure similar to the influence of impurities and defects. This means that H did not influence the electron motion but disturbed the structure of the lattice-site bonds through magnetoelastic stresses, thus modifying the conduction electron energy state. The methods for application of model presentation based on the quantum mechanics were discussed in parallel. The notions relating to classical mechanics (elasticity, magnetoelasticity) that explained real physical processes in the kinetics of microprocesses had not been developed properly. This also concerned the investigations under hydrostatic pressures. The use of quantum mechanics causal basis has resulted in generalizing theories with numerous parameters.

The followed the investigation of galvanomagnetic phenomena using the methods of hydrostatic pressure generation [208, 209]. The pressure varied the structure parameters and resulted in phenomena related to the electron density change as well as to typical anomalies in thermodynamic and kinetic

processes. The mechanisms of continuous lattice deformation stimulated the deforming stresses similar to T and H effect.

The complexity of the procedure depends on the object of the investigation. For a metal, the elastic compression modulus equals to 10^{-6}, this is identical to P~100 kbar and the pressure of 1-2 kbar is commensurate, the effect is low and as a consequence, the pressures about 30 kbar should be generated to determine the regularities.

In [210, 211], a series of materials such as Sn, Zn, Pb, Hg, Al, Cd, Nb has been investigated. They are typical of the regular change of the crystal temperature T_c with phase transition and dT_c/dP with the minus sign is considered to be the second-order phase transition. For La, Ti, Zr, V, dT_c/dP varies with plus sign that is the first-order phase transition.

While analyzing the properties of tin, indium, lead and tantalum with identical tendencies of the pressure effect corresponding to the second-order phase transition [212], we paid attention to an unusual change of the phase transition in Thallium (Fig. 9.4a). At the initial stage of the temperature shift to 0.02^o, for P to 7 kbar, T(P) varies non-monotonously in view of the measurement error for a shelf-like dependence. Subsequent dT/dP changes with the minus sign are typical of the second-order phase transition. Using the results of [6], we defined the critical point P_x indicating the position of the structural second-order phase transition and place $T_p(P)$ in correspondence with the position of P_x with respect to the temperature change (Fig. 9.4b) clockwise. For P under 30 kbar, the non-linear component shows the sign change region for the priorities of thermoelastic effect of baroresistivity as well as the role of properties in the formation of elastic anisotropy of the electron density. The influence of impurities results in structure changes and the evolution of the state of electron density. This can be followed by barotemperature dependence of the second-order phase transition [213, 214]. For the structural phase transition, this regularity of $LaMnO_3$ magnetostriction properties is unambiguous (Fig. 7.2 of [6]).

For this metal, the mentioned pressures realize the mechanisms of elastic stresses corresponding to the values of the compressibility factor of 10^4 (10^{-6}-10^{-7}) which is insignificant for this method of investigations. But the observed tendency reflects the state of the second-order phase transition and the dependence of Fig. 9.4a is due to both the deforming influence of the stresses on the structure affecting PT formed to 0 K and to the consequence of the conduction-electron density change in the metallic phase.

Under 30 kbar, the non-linear component reflects the conformity of the pressure effect on the structure changes similar to the effect of impurities of the dynamics of the changes and PT formation and, as a consequence, the formation of the properties and the phase states.

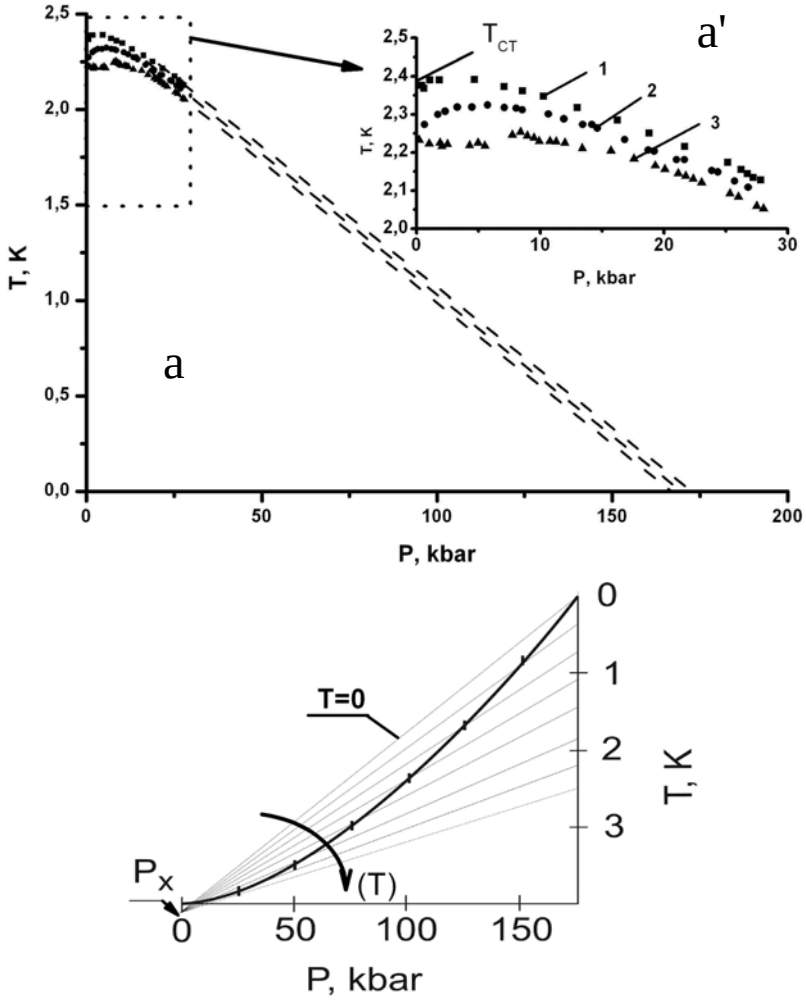

Figure 9.4. (a) Temperature and pressure dependence of the phase transition in Tl (1) doped by Hg (0.45%) (2) and Hg (0.9%) (3). (b) Temperature and pressure dependence of the phase transition in Tl with the separated critical point P_x: $T_{pp}=T_{mc}$~2.4 K, $T_x=T=0$, P_x~160 kbar.

The application of pressures has determined the relationship and analogy between the structure changes and the topology of the spectrum of phase-state electron density and the impurity concentrations. The distinguished crystallographic anisotropy apparent in the mechanisms of elastic stresses is a phenomenon of the shape.

While considering the superconducting phase state through the dependence dT_p/dP with the positive sign, we see that the pressure influencing the structure changes and varying the parameters is a factor bringing the system and the magnetoelasticity to the metallic phase state.

The pressure and the magetnostriction are factors changing the shape and the volume at the expense of baro- and magnetoelasticity exactly due to bulk elastic stresses. The factor of elasticity anisotropy is the defining one in the changes of the topology of the phase state electron density on the background

of the structural phase transition. It is the dependence of the magnetic field effect on the structure, that develops the changes of the magnetic susceptibility in cadmium, beryllium, magnesium, tin, indium single crystals through the magnetoelastic mechanisms.

The analysis of the results and the fact of distinguishing the linear law of the resistance change (Kapitsa) make us to state that the electron mobility induced by the magnetic field is connected with the crystal structure disturbances which affect the conductivity in a way similar to impurities or defects. In the low-temperature range, the magnetic field affects the structure of atomic bonds or the whole lattice that is the primary reason of the influence on the electron mobility. The changes of the field direction are related to the fact of distinguished directions of magnetic non-compensation in the structure. As a consequence, the direction of the disturbance is changed due to the anisotropy of magnetic properties and magnetic elasticity.

9.3. Structural phase transition in ferroelectrics in varied T and P parameters

The studies of the critical phenomena in the processes of structure rearrangements under T and P effects are not simple because researches are scare and the results are doubtful. The correlation between the parameters of the changes conforms the temperature and pressure dependences. Thus, for a ferroelectric $BaTiO_3$ [215], dT/dP equals 8.4 K/kbar, and dT/dP makes 5.1 K/kbar in manganates $La_{0.7}Ca_{0.3}MnO_3$ [6], the compressibility is good. At the same time, dT/dP equals 0.37 K/kbar for EuO during the ferromagnetic transition [216], i.e. the structure changes under the influence of dT/dP with the positive sign are a first-order structural phase transition with a high enough hysteresis. The regularity is also typical of $CaCl_2 \cdot 2H_2O$ [6] with 0.33 K/kbar and dH/dP of 1.34 kOe/kbar.

A non-trivial grounding of the investigations of the critical phenomena in systems of the perovskite family differs much from ferroelectric phase transitions with the compressibility of ~ 10^{-3}-10^{-4} found experimentally because of multi-component system and coefficient of Om compressibility of 10^{-6}as well as because of the instability at the boundaries of the phase states. The most reliable results give methods of the elastic neutron scattering and resonance methods.

The structural phase transition is considered to be a reversible physical process where non-uniformities and the strong bond between the structure parameters and elastic stresses are reflected in the smearing of the phase transition and in the shift of phase transition temperature T, consequently.

It is the difficulty of interpretation of the experimental results that does not permit us to distinguish and to predict the state of structural changes in

processes of stress strain under the PT and to provide an adequate model theoretical grounds that take the real physical process into account. In this process, changes of the volume and the energy of bulk elasticity are not completely considered by classical theories which treat the phase states.

Analyzing the position of the critical states for perovskite family where the parameters at the phase transition boundary are unstable $T_{mc}=T_{pp}$ [6] and correspond to the second-order phase transition with the critical points P_x and PP_x, it is noted that these critical points distinguished from regular changes of magnetostriction properties determine the phase state under P and H effect through baroelasticity and magnetoelasticity mechanisms. The mentioned regularities propagate to the physical properties of PT realization to temperatures T=0 K [217, 218]. Analogous results of Figs. 9.5ab for a mixed $Kta_{1-y}Nb_yO_3$ system [219] help in application of the results of [6] qualitatively to study the second-order PT and properties of ferroelectrics.

In the crystal, the presence of imperfections is the most obvious in the dynamics near critical points. To classify the processes, we need differentiate between the principal and the minor things. The main item is the determination of the causal basis for the elasticity mechanisms realized during the development of the structural phase transitions as well as the analogies for the defining role of parameters T-H-P through thermo-, magneto- and baroelasticity that result in PT and structure changes. It is also important to consider the same mechanisms under the formation of discontinuous structural phase transitions giving bulk and symmetry changes, anomalous hysteresis, i.e. resulting in the first-order structural phase transitions at 0 K where quantum-mechanical grounds are not important for the critical region [200].

In thee presence of defects, the nature of the critical phenomena is followed in the dynamics of property changes in the vicinity of the critical points due to the mechanisms that form the phenomena. A physical process could hardly be modeled without the critical phenomena.

The process of experimental analysis has not been finished yet. The nature of the mechanisms forming the critical phenomena in ferroelectrics still remains not properly understood. It sees highly interesting to make an experiment to study samples under high hydrostatic pressure with varying T and H and to analyze the results basing on the existing preconditions for relationship between the bulk elasticity, structure and properties.

The regularity of quasi-elastic phenomena such as the elastic stresses and the elasticity anisotropy is the basis of current understanding of the dynamics of the critical phenomena in the vicinity of the structural shift-type phase transitions. No matter how paradoxical it is, the developed theoretical representations are not considered from such a viewpoint, and now it is even hard to conceive how these mechanisms can characterize changes in perfect crystals.

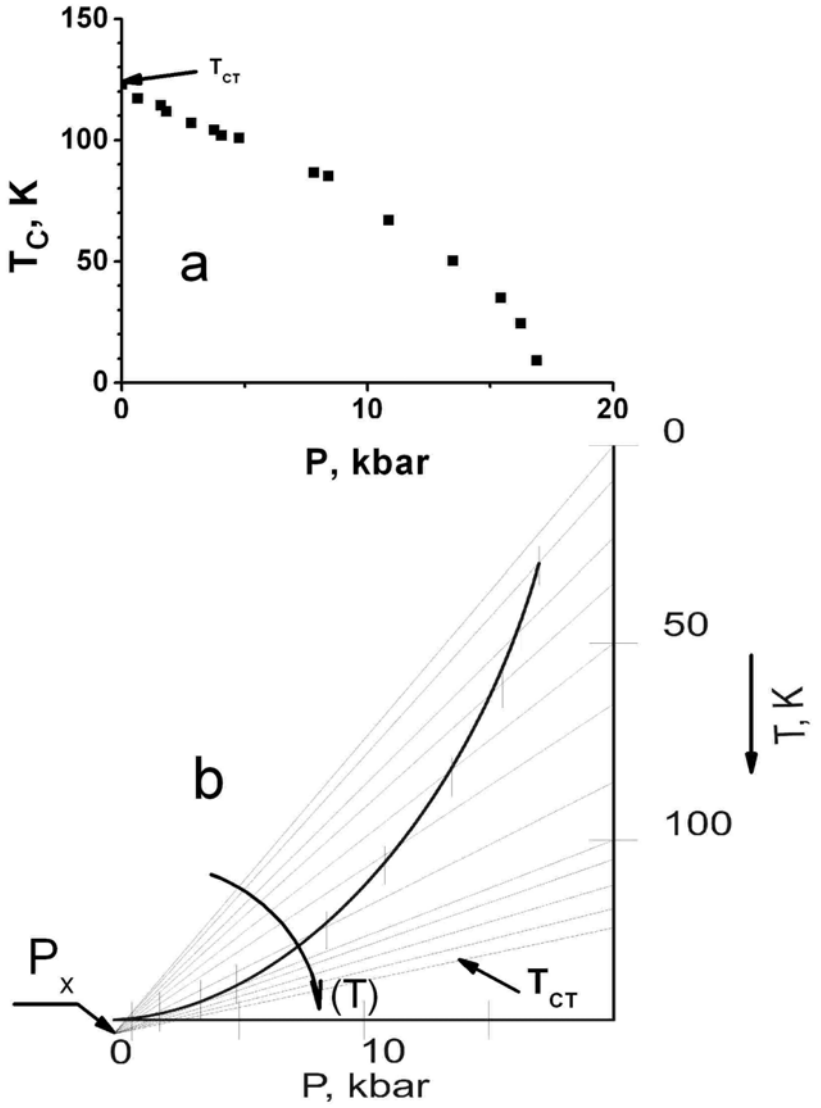

Figure 9.5. (a,a') Temperature and pressure dependence of the phase transition in a ferroelectric in KDP [219]. (b) Temperature and pressure dependence of the structural phase transition of the second order with the separated critical point P_x and $T_{pp}=T_{mc}$~122 K, $T_x(T=0)$, P_x~17 kbar.

9.4. Conclusions

While studying a complex state of material, a researcher faces a great amount of information without proper treatment of the results. The empirical principles are not formulated correctly that does not contribute to the understanding of reality. A very complex task of a researcher is the control of intuition that allows one to distinguish sign of objective universality. Otherwise, it is impossible to suggest a real model of the studied physical process where any quantitative changes do not influence the basic physical principles forming the structure of a solid and cover a wide variety of macro- and microscopic properties of the studied system.

Now we shall evaluate the levels of energy contribution in the course of consideration of critical phenomena and properties. This matter touches upon principal questions of the direct relation between thermodynamic parameters and structure evolution through the mechanisms of elastic stresses affecting the volume and other parameters controlling the structural phase transitions and the properties of phase states.

We shall estimate the energy of Coulomb interactions as 1÷10 eV, the influence of the crystal field as 0.1÷1 eV, spin-orbit relationship as 10^{-2}÷10^{-1} eV, spin-spin (magnetic) bond as 10^{-4} eV, electron-nuclear bond as 10^{-4}÷10^{-5} eV. According to our estimations, the energy of elastic stresses with taking into account the coefficient of compressibility is 1÷10 eV.

The magnetism of magnet-containing structures can get the most effective consideration from the viewpoint of the experiment. There the real physical process is registered if the form of the evolution of the properties of a solid that testifies the regular bond of the changes of the crystal structure and the electronic and magnetic properties.

Model representations treat the energy to a first approximation without sensibility to phase transitions. Directly calculating the energy, the models do not pay proper attention to magnetoelastic interactions and magnetization.

We should keep in mind that magnetoleastic interactions are nothing but bulk striction based of the elastic bond between neighbor non-compensated spins. Thus, all changes of interatomic distances result in both the changes of the volume and the lattice form followed by the modification of the properties.

Magnetization is a consequence of the influence of the magnetic field on magnetically non-compensated constituent of a particle provided it is high enough to affect the structure significantly.

We should take into account that quantum mechanical forces forming the magnetism are of short range in fact, so deep understanding of the regularity if interaction is necessary for the estimation of this process.

The elastic energy is an immediate energy of long range. These are elastic stresses in the structure that form the linearity of the magnetization regardless of important details of microscopic interactions. By definition, atoms and molecules have small magnetic moments of non-compensation. The structure is the totality of molecules and atoms brought into the sites of the structure (several atoms and molecules) and bound in the lattice by the compatibility of valent and free electrons.

The state of the structure and its predisposition to paramagnetism is formed by high-temperature physical and chemical processes where the magnetic factor is absent by definition. In other words, the high-temperature area has no ability for magnetization.

The succeeding cooling and bulk compression result in the loss of heat energy transformed into the loss of the energy of the elastic stresses in the structure. This process is followed by the linear evolution of the parameter due to the mechanisms of bulk elasticity.

This process is the factor forming the spin non-compensation of sufficient intensity at the proper state of the structure that allows the structure to react on the magnetoelasticity and magnetization in the applied magnetic field. These are the approaches of the analysis that permit to define the causal role of the laws of bulk elasticity in the formation of the magnetism as well as their leading role in the first and second order structural phase transitions.