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Microscopic theory of magnetic-field-induced structural phase transitions

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The microscopic theory of a magnetic-field-induced structural phase transition is developed. The mechanism of the phase transition is connected with the cooperative Jahn-Teller effect. For a set of microscopic parameters determined earlier the anomalies in the acoustic, magnetic, and magnetoelastic properties have been analyzed for a wide range of temperature and external magnetic fields. Special attention is paid to the unusual giant dynamic magnetostriction. [S0163-1829(97)04633-X]

INTRODUCTION

The understanding of the mechanism of the cooperative phenomena in condensed matter at a microscopic level remains of prime importance in many modern fields of science including ferroelectricity, superconductivity, magnetism, structural transformations, polymerization, peptide folding, and others. In this list, the structural phase transitions are of special and very visible significance for being tightly connected to the electronic structure and influencing the properties of the matter.

Nowadays the most developed microscopic theory of structural transformations is based on the analysis of the electron-phonon interaction which in the case of the non-Kramers degeneracy of the electronic subsystem is often called the cooperative Jahn-Teller effect. The applications of this theory to the modern problems mentioned above is under consideration in numerous recently published articles and books.[1–8] It is completely clear that if the Jahn-Teller effect is really responsible for the structural transition in the system under consideration, the external magnetic field, while influencing directly only the electronic subsystem, can drastically effect the geometry of the distribution of nuclei in space (the crystal lattice in the case of solids). Therefore the magnetic-field influence on structural transitions can be considered as a positive test for the electron-phonon microscopic mechanism.

The changes in the properties of Jahn-Teller ferroelastic crystals caused by the external magnetic fields were considered earlier in many papers (see Ref. 9, and references therein). However in this paper we are analyzing a phenomenon of structural phase transition induced by the magnetic-field-stimulated cooperative Jahn-Teller effect.[10,11] As contrasted with the previously analyzed systems in the crystals under consideration no phase transitions take place without magnetic field, so that there are no doubts as to the electron-phonon origin of the phase transitions. Recently such structural phase transitions were observed in the experiments on giant magnetostriction[12] and on Raman scattering.[13] Below, the theory of the magnetic-field structural transitions is analyzed in detail by using the $\mathrm{TmPO_4}$ and $\mathrm{Tb}_x\mathrm{Y}_{1-x}\mathrm{VO}_4$ crystals as examples. The results of numerous calculations of different crystal properties, already experimentally observed or predicted, are presented.

THE HAMILTONIAN

The crystals under consideration have the tetragonal zircon structures D_{4h} and the local symmetry of the rare-earth Jahn-Teller ions is D_{2d}. The $\mathrm{TmPO_4}$ and $\mathrm{Tb}_x\mathrm{Y}_{1-x}\mathrm{VO}_4$ crystals are the representatives of this class of materials. The electronic structure of the Tm^{3+} and Tb^{3+} ions is described by two singlets separated by a 2Δ gap, in the middle of which there is a non-Kramers doublet. Other energy levels are well separated from this ground group and are not considered at the low temperatures of interest. This is done because at these temperatures only the induced structural phase transitions take place. In this case the higher energy levels are practically empty. At the same time, the mixing of these excited states with the ground quadruplet can be ignored because, at the magnetic field under consideration, the Zeeman energy is much smaller than the energy gap between these two groups of levels.

The Hamiltonian of the crystal with this electronic basis can be written as[8]

$$H=H_{\text{el-ph}}+H_{\text{el-str}}+H_{\text{ph}}+H_{\text{str}}+H_{\text{cryst}}+H_{\text{Zeem}}, \tag{1}$$

where

$$H_{\text{el-ph}}=\sum_{m\kappa} V_{m\kappa}\sigma_z^m(b_\kappa+b_{-\kappa}^+),$$

$$H_{\text{el-str}}=-g_0\sqrt{\frac{C_0\Omega}{N}}\,U_z\sum_m \sigma_z^m,$$

$$H_{\text{ph}}=\sum_\kappa h\omega_\kappa\left(b_\kappa^+b_\kappa+\frac{1}{2}\right),\quad H_{\text{str}}=\frac{1}{2}C_0\Omega U_z^2, \tag{2}$$

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$$H_{\mathrm{cryst}}=-\frac{\Delta}{2}\,(1+\tau_z)\sigma_x\,,$$

$$H_{\mathrm{Zeem}}=-g\beta\sum_m\,(H_xS_x^m+H_yS_y^m).$$

In Hamiltonian (1) the first two terms describe the interaction of the electrons with the phonons (the second quantization operators b_κ, b_κ^+) and the homogeneous strain U_z, the next two terms are connected with the free phonons and homogeneously strained crystal elastic energy, and, at last, the last two terms represent the crystal-field splitting of the electronic states (singlet-doublet-singlet structure) and the Zeeman interaction with the $x\|a$ and $y\|b(=a)$ components of the external magnetic field. It is important that the magnetic-field orientation at 45° to the crystal a axis,

$$\left(H_x=H_y=\frac{1}{\sqrt{2}}\,H_0\right),$$

will be under consideration in this paper. The magnetic field H_z perpendicular to the ab plane of the crystal can only suppress the orthorhombic strain in the D_{4h}-symmetry tetragonal crystals.[8] At $H\|[110]$ or $[010]$ the magnetic field forms the crystal strain of $B_{2g}(D_{4h})$ symmetry due to the regular magnetostriction effect, according to symmetry group theory. That strain symmetry is the same as the spontaneous strain at the induced structural phase transition. In other words, at this field orientation the strain exists at any nonzero magnetic field, so that no phase transitions can occur. At $H\|[110]$, (45° to the crystal a-axis orientation), the $B_{2g}(D_{4h})$ strain cannot be induced as regular magnetostriction, and its appearance is the result of the cooperative interactions. This is discussed below in greater detail in the discussion of magnetostriction.

The matrices of the electronic operators at a chosen basis can be represented as

$$\sigma_z=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{pmatrix},$$

$$\frac{1}{2}\,(1+\tau_z)\sigma_x=\begin{pmatrix}0&0&1&0\\0&0&0&0\\1&0&0&0\\0&0&0&0\end{pmatrix},\qquad(3)$$

$$S_x=\frac{1}{2}\,(1+\sigma_z)\tau_x=\begin{pmatrix}0&1&0&0\\1&0&0&0\\0&0&0&0\\0&0&0&0\end{pmatrix},$$

$$S_y=\frac{1}{2}\,(1-\sigma_z)\tau_x=\begin{pmatrix}0&0&0&0\\0&0&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix}.$$

We note that σ and τ matrices are similar to the Dirac matrices for the electron, and obey the commutation rules[14]

$$\sigma\times\sigma=2i\sigma;\quad \tau\times\tau=2i\tau;\quad [\sigma,\tau]=0.\qquad(4)$$

It is easy to see after the minimization of the crystal energy upon the spontaneous U strain that the last relation is proportional to the average of the S_z electronic operator

$$U_z=g_0\sqrt{\frac{N}{C_0\Omega}}\,\sigma_z\qquad(5)$$

(the spontaneous strain U_z is the order parameter and has the B_{2g} symmetry as the structural phase transition is from tetragonal symmetry to the orthorhombic D_{2h} symmetry).

For further analysis of the Hamiltonian (1) it is convenient to subject it to a unitary shift transformation $H=\exp(iR)H\exp(-iR)$,[15,16] where

$$R=\sum_m\,g_m\sigma_z^m,\quad g_m=i\sum_\kappa\,\frac{V_{m\kappa}}{h\omega_\kappa}\,\sigma_z^m(b_\kappa^+-b_\kappa).\qquad(6)$$

After the transformation the crystal Hamiltonian takes the form

$$H=H_{\mathrm{el\text{-}str}}+H_{\mathrm{str}}+H_{\mathrm{ph}}+H_{\mathrm{Zeem}}-\sum_{mn\kappa}\,\frac{V_{m\kappa}^*V_{n\kappa}}{h\omega_\kappa}\,\sigma_z^m\sigma_z^n$$
$$-\frac{1}{2}\,\Delta\sum_m\,(1+\tau_z^m)(\sigma_x^m\,\cos 2g_m-\sigma_y^m\,\sin 2g_m).\qquad(7)$$

The fifth term of the transformed Hamiltonian (7) describes the virtual phonon exchange of the Ising type responsible for the effective electron-electron interaction in the crystal, the first four terms are unaffected by the transformation as the corresponding operators commute with the shift operator (the free-phonon operators describe the same frequency phonons with the shifted equilibrium positions). The last term of Eq. (7) has a complicated form (the price for the accurate Hamiltonian transformation of the system under consideration) and represents the dynamical coupling of the electron and phonon variables. Separating the electron variables from the phonon variables (the k-space area of strong dynamic interaction is much smaller than the size of the first Brillouin zone) for the electronic part of the Hamiltonian one obtains

$$H_{\mathrm{el}}=-\sum_{mn}\,A_{mn}\sigma_z^m\sigma_z^n-\frac{1}{2}\,\Delta\gamma(1+\tau_z^m)\sigma_x^m$$
$$-\frac{1}{\sqrt{2}}\,g\beta H\sum_m\,(S_x^m+S_y^m),\qquad(8)$$

where

$$A_{mn}=\sum_\kappa\,\frac{V_{m\kappa}^*V_{n\kappa}}{h\omega_\kappa}\,\sigma_z^m\sigma_z^n+g_0^2\sigma_z\sum_m\,\sigma_z^m\qquad(9)$$

is the effective electron-electron interaction constant where the contribution of the electron-strain interaction is taken into account. It is seen in Eq. (9) that the interelectronic interaction in the Jahn-Teller crystals is the result of the virtual phonon exchange and the interaction of the electrons with the homogenous strains. In this case, the effective electron correlation radius depends on the wavelength of the phonons which contribute to the interaction. In the $TmPO_4$ and $TbVO_4$ crystals, the greatest contribution to A_{mn} comes from the long-wavelength acoustic phonons and the homogeneous strains (infinitely big wavelengths). Therefore the correlation radius is big, and that is confirmed experimentally.[8] On the other hand, it is well known that the molecular field approximation is valid if the crystal lattice constant a is smaller than the correlation radius r. At $a/r \ll 1$ the molecular field approximation describes the system quantitatively, (see Chap. 3 in Ref. 8, and references therein).

As the systems under consideration are characterized by the long-range radius of correlations the molecular field approximation is good enough for a quantitative analysis of the properties of the crystals. In this approximation the electronic order parameter σ is described by the following equation:

$$\sigma_z=\frac{A\sigma_z/\sqrt{a+\sqrt{b}}(1+h_0^2/\sqrt{b})\sinh(\sqrt{a+\sqrt{b}}/kT)+A\sigma/\sqrt{a-\sqrt{b}}(1-h_0^2/\sqrt{b})\sinh(\sqrt{a-\sqrt{b}}/kT)}{\cosh(\sqrt{a+\sqrt{b}}/kT)+\cosh(\sqrt{a-\sqrt{b}}/kT)}, \tag{10}$$

where

$$a=A^2\sigma_z^2+\Delta^2\gamma^2+\frac{1}{2}h_0^2;\quad b=\Delta^4\gamma^4+\frac{1}{2}h_0^2(\Delta^2\gamma^2+4A^2\sigma_z^2),\quad h_0=g\beta H. \tag{11}$$

Taking into account that $2(a+\sqrt{b})$ is the gap between the ground and the excited singlets and $2(a-\sqrt{b})$ is the splitting of the doubly degenerate (at $H=0$) excited state, Eq. (10) can be written as

$$\sigma_z=P_1\frac{A\sigma_z(1+h_0^2)\tanh(\sqrt{a+\sqrt{b}}/kT)}{\sqrt{a+\sqrt{b}}}+P_2\frac{A\sigma_z(1-h_0^2)\tanh(\sqrt{a-\sqrt{b}}/kT)}{\sqrt{a-\sqrt{b}}}, \tag{12}$$

where

$$P_1=\frac{\cosh(\sqrt{a+\sqrt{b}}/kT)}{\cosh(\sqrt{a+\sqrt{b}}/kT)+\cosh(\sqrt{a-\sqrt{b}}/kT)} \tag{13}$$

is the total population of the singlet states and $P_2=1-P_1$ is the total population of the doublet components.

If the electronic order parameter σ from Eq. (10) or (12) is not zero the spontaneous strain U_z according to Eq. (5) is also nonzero and the structural phase transition takes place. It is easy to see that in the case of $H_x=H_y=0$, Eq. (10) and the population P_1 are given by expressions discussed earlier[17]

$$\sigma_z=\frac{A\sigma_z/(\sqrt{A^2\sigma_z^2+\Delta^2\gamma^2})\sinh(\sqrt{A^2\sigma_z^2+\Delta^2\gamma^2}/kT)+\sinh(A\sigma_z/kT)}{\cosh(\sqrt{A^2\sigma_z^2+\Delta^2\gamma^2}/kT)+\cosh(A\sigma_z/kT)}, \tag{14}$$

$$P_1=\frac{\cosh(\sqrt{A^2\sigma_z^2+\Delta^2\gamma^2}/kT)}{\cosh(\sqrt{A^2\sigma_z^2+\Delta^2\gamma^2}/kT)+\cosh(A\sigma_z/kT)}. \tag{15}$$

The transcendental equation (14) at $H=0$ was analyzed in Ref. 14, where it was shown that for $\Delta/A>1.20$ only one solution exists at $\sigma_z=0$. This is the case of the $TmPO_4$ crystal where $\Delta/A=1.33$ and no phase transitions take place at all temperatures. This also holds for different compositions of sufficiently diluted $Tb_xY_{1-x}VO_4$ crystals. However, we have found that in the presence of sufficiently big magnetic fields oriented at 45° to the crystal a axis, $\sigma\neq 0$ solutions exist. Moreover, at some values of magnetic fields two structural phase transitions take place. The second reentrant phase transition corresponds to the return of the crystal from the orthorhombic phase to the higher-symmetry tetragonal phase with the lowering temperature.

The calculations of the crystal phase diagrams dependence upon the external magnetic fields were done in Ref. 18. Here we will focus mostly on the physics of the induced structural transformations and accompanying these transformations, anomalies of different crystal properties.

The microscopic mechanism of the structural phase transitions under consideration can be understood in the framework of the general theory of the cooperative Jahn-Teller effect. According to that approach the structural phase transition is the result of the electron-phonon interaction and of the corresponding virtual phonon exchange in the cooperative systems. However, in the pseudo-Jahn-Teller crystals, where the vibrations mix initially split energy levels, the phase transition takes place only when the electron-electron correlations are bigger than the initial energy gap. In the $TmPO_4$ crystal the virtual phonon exchange interaction, while not zero, is not sufficiently great to overlap the energy gap ($A=22.5\ \mathrm{cm}^{-1}$, $\Delta=30\ \mathrm{cm}^{-1}$) and as a result there are no phase transitions. But if the external magnetic field $H_x=H_y$ is not zero, the phase transitions can be induced if the field value is greater than some critical value. This can be interpreted in the following way. The external H field affects the system in two ways: it changes the energy gaps between

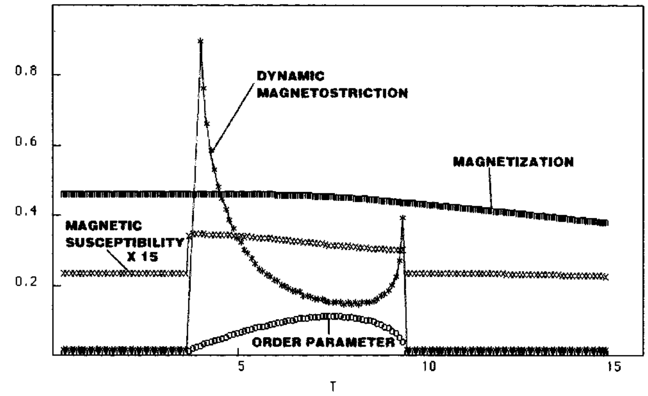

FIG. 1. The order parameter, dynamic magnetostriction, magnetization, and magnetic susceptibility as a function of temperature for parameters $\Delta = 30$, $A = 22.5$, and $h = 17.7$. All units are in cm^{-1}. The parameters Δ and A correspond to $\mathrm{TmPO_4}$.

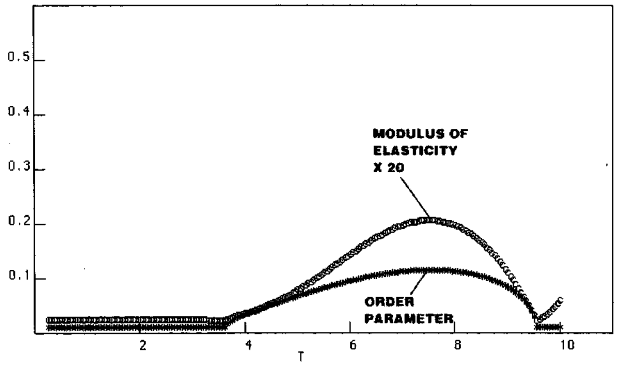

FIG. 3. The order parameter and the modulus of elasticity as a function of temperature for parameters $\Delta = 30$, $A = 22.5$, and $h = 17.7$. All units are in cm^{-1}. The parameters Δ and A correspond to $\mathrm{TmPO_4}$.

the electronic states and it changes the electronic wave functions mixing each of the singlet components with one of the doublet components. This can be easily seen from the structure of the electronic operators of the magnetic moments $M_x = g\beta S_x$ and $M_y = g\beta S_y$. Calculations show that the mixing of the wave functions is very important for the effectiveness of the electron-electron interaction.

It is worthy of note that such magnetic-field influence on systems with structural phase transitions is quite unusual. In all previously analyzed systems under the external magnetic field, the field could only reduce the phase transitions or smear out them. Which effect actually took place depended upon the symmetry properties of the solids, on the magnetic fields, and upon the commutation rules of the operators of the electron-phonon and Zeeman interactions. The magnetic-field-induced structural transitions are connected with a new situation that will be discussed in the section dealing with the magnetoacoustic properties.

ORDER PARAMETER

The order parameter σ is described by Eqs. (12) and (14) which are valid at all temperatures and all values of the magnetic fields. These equations are transcendental equations and their numerical solutions are represented in Figs. 1–8. It can be seen that depending upon the Δ/A ratio, temperature, and magnetic field, one, two, or no structural phase transitions are found. In some cases the $\overline{\sigma_z} \neq 0$ solution for some temperatures appears only at $H_0 \neq 0$. This corresponds to field-induced transitions. The two transitions correspond to the reentrance of the crystal from a low-symmetry to a high-symmetry phase as the temperature of the system is lowered. Such a possibility for diluted $\mathrm{Tb}_x\mathrm{Y}_{1-x}\mathrm{VO}_4$ crystals was discussed earlier.[14] We show here that the reentrant phase transitions can also be induced by the external magnetic fields.

For analysis of the magnetic-field influence on the order parameter let us consider the order parameter equation at $T=0$. As it follows from Eqs. (13) and (14), at zero temperature $P_1 = 1$, $P_2 = 0$ and

$$\overline{\sigma_z} = \frac{A\overline{\sigma_z}}{\sqrt{a+\sqrt{b}}}\left(1+\frac{h_0^2}{\sqrt{b}}\right). \tag{16}$$

From this equation it is easy to find the critical magnetic-field value at which the structural phase transition takes place at $T=0$. For $h_{0\,\mathrm{crit}}$ we find the equation

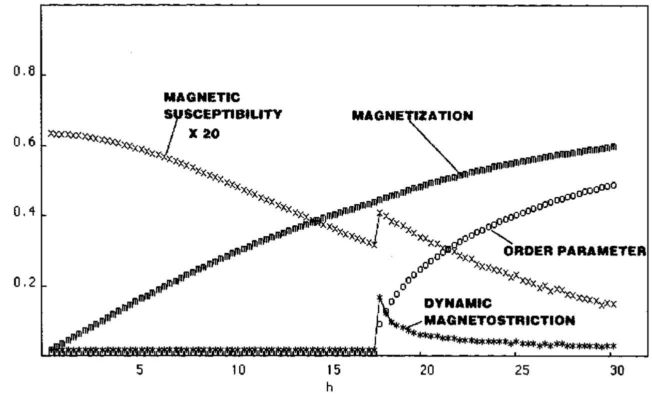

FIG. 2. The order parameter, dynamic magnetostriction, magnetization, and magnetic susceptibility as a function of the magnetic field h, for parameters $\Delta = 30$, $A = 22.5$, and $T = 8.7$. All units are in cm^{-1}. The parameters Δ and A correspond to $\mathrm{TmPO_4}$.

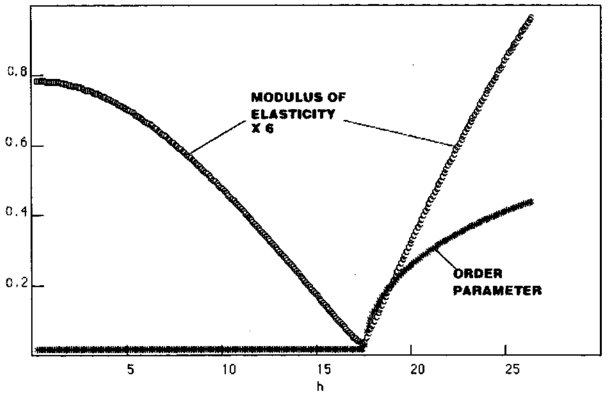

FIG. 4. The order parameter and the modulus of elasticity as a function of the magnetic field for parameters $\Delta = 30$, $A = 22.5$, and $T = 8.7$. All units are in cm^{-1}. The parameters Δ and A correspond to $\mathrm{TmPO_4}$.

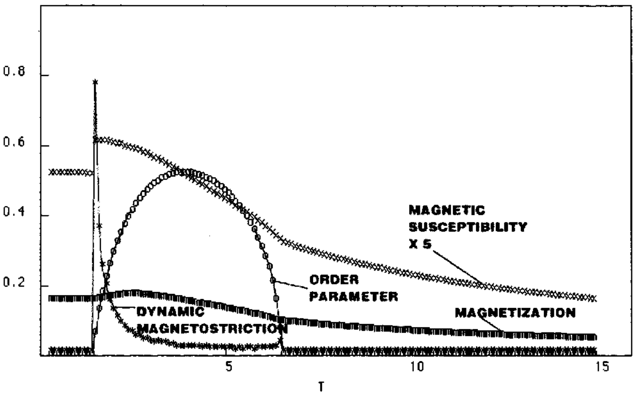

FIG. 5. The order parameter, dynamic magnetostriction, magnetization, and magnetic susceptibility as a function of temperature for parameters $\Delta=9$, $A=8.65$, and $h=1.44$. All units are in cm^{-1}. The parameters Δ and A correspond to $\mathrm{Tb}_x\mathrm{Y}_{1-x}\mathrm{VO}_4$.

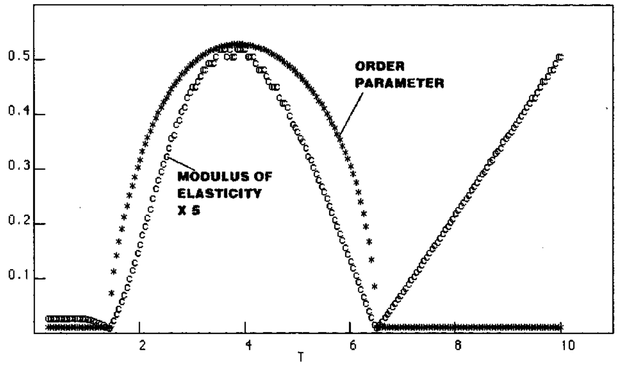

FIG. 7. The order parameter and the modulus of elasticity as a function of temperature for parameters $\Delta=9$, $A=8.65$, and $h=1.44$. All units are in cm^{-1}. The parameters Δ and A correspond to $\mathrm{Tb}_x\mathrm{Y}_{1-x}\mathrm{VO}_4$.

$$\frac{1}{A}=\frac{1+2h_{0\,\mathrm{crit}}^2/\Delta^2\gamma^2\sqrt{1+2h_{0\,\mathrm{crit}}^2/\Delta^2\gamma^2}}{\sqrt{h_{0\,\mathrm{crit}}^2/2+(\Delta^2\gamma^2/2)(1+\sqrt{1+2h_{0\mathrm{crit}}^2/\Delta^2\gamma^2})}}. \qquad (17)$$

From Eq. (17) it is seen that at $h_{0\,\mathrm{crit}}=0$ the structural phase transition is possible only if $A=\Delta\gamma$. However if the magnetic field is present the solutions of Eq. (17) exist even for $\Delta\gamma>A$ as is shown in Figs. 1–8. In part, it follows from Eq. (17) that at $h_0\rightarrow\infty$ the solution of Eq. (17) exists if $A=1/2\Delta\gamma$. The meaning of this result is that while the magnetic field makes possible the structural phase transition even at $\Delta\gamma>A$, nevertheless the crystal field splitting cannot be bigger than double the molecular Jahn-Teller field. If it is, the phase transition does not take place at any magnetic field.

MAGNETOSTRICTION

It is well known that magnetostriction is the phenomenon of inducing or changing the strain of a sample by means of an external magnetic field. In that sense the induced structural phase transition is a magnetostriction effect. However, it is a very unusual magnetostriction. As a rule the magnetostriction is quadratic in magnetic fields when they are small. This is a direct result of the symmetry of the strain and of the magnetic-field orientation. The square of the magnetic-field symmetry representation contains the symmetry representation of the strain that causes the coefficient of proportionality between the strain and the magnetic field square to be nonzero. However this is not the case in the phenomenon of the induced structural phase transitions. For crystals with zircon structure the square of the representation of the magnetic field oriented at 45° to the crystal a axis ($A_{1g}+B_{1g}$ representations) does not contain the B_{2g}-symmetry representation of the spontaneous strain. As it is seen from Figs. 1–8 the strain does not depend upon the magnetic field remaining zero if $H_0<H_{\mathrm{crit}}$, and even at the bigger fields, when the strain is induced, the dependence upon the magnetic field is not quadratic. Moreover, the regular magnetostriction upon the field dependence is characterized by the presence of a knee before the striction saturation starts. As it can be seen from our calculations no knees are present at the induced structural phase transition phenomenon.

Other much more drastic changes of the magnetostriction under consideration in comparison with the regular one are connected with the dynamic magnetostriction. Figures 1, 2, 5, and 6 show a strong maximum near the structural phase transition. From the first point of view this result is not as surprising as earlier, the giant dynamic magnetostriction in

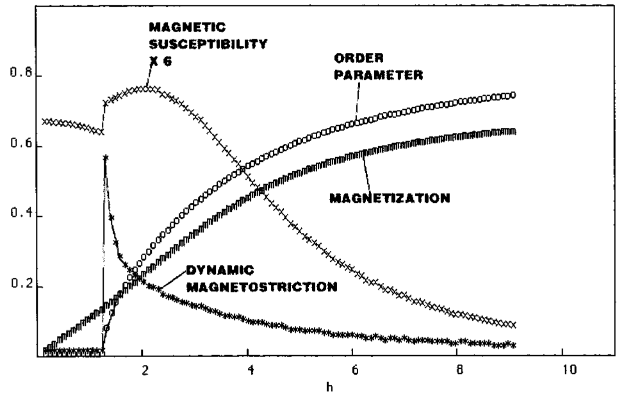

FIG. 6. The order parameter, dynamic magnetostriction, magnetization, and magnetic susceptibility as a function of the magnetic field h, for parameters $\Delta=9$, $A=8.65$, and $T=1.53$. All units are in cm^{-1}. The parameters Δ and A correspond to $\mathrm{Tb}_x\mathrm{Y}_{1-x}\mathrm{VO}_4$.

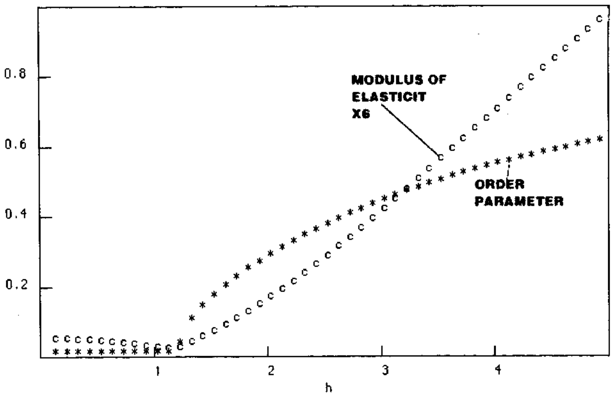

FIG. 8. The order parameter and the modulus of elasticity as a function of the magnetic field h, for parameters $\Delta=9$, $A=8.65$, and $T=1.53$. All units are in cm^{-1}. The parameters Δ and A correspond to $\mathrm{Tb}_x\mathrm{Y}_{1-x}\mathrm{VO}_4$.

the paramagnetic ferroelastics was predicted theoretically and observed experimentally. However, in comparison even with the giant dynamic magnetostriction of the cooperative Jahn-Teller crystals, the magnetostriction under consideration is qualitatively different. The dependence of the width of the peak of the dynamic striction upon the field dependence is very narrow, much narrower than in the earlier discussed situations. For example, in the same TmPO_4 and $\mathrm{Tb}_x\mathrm{Y}_{1-x}\mathrm{VO}_4$ crystals under external magnetic field $H \| a$, the discussed peak is broadened as a result of the smearing out of the structural phase transitions when they exist without the field. But at the 45° orientation of the field no smearing out of the transition takes place and that is why the peak of the dynamic magnetostriction is narrower.

MAGNETIC PROPERTIES

Magnetic properties of the Jahn-Teller crystals with structural phase transitions are very specific. It is reasonable to expect for these properties some specific anomalies connected with the induced phase transitions.

In the framework of the developed approach the magnetic moment M parallel to the H_0 field is proportional to the average of the electronic operator S_0 which is described by the formula

$$\overline{S_0}=\frac{1}{2}\,h_0\,\frac{[1+(4A^2\overline{\sigma_z^2}+\Delta^2\gamma^2)/2\sqrt{b}]/\sqrt{a+\sqrt{b}}\,\sinh(\sqrt{a+\sqrt{b}}/kT)+(1-4A^2\overline{\sigma_z^2}/2\sqrt{b})/\sqrt{a-\sqrt{b}}\,\sinh(\sqrt{a-\sqrt{b}}/kT)}{\cosh(\sqrt{a+\sqrt{b}}/kT)+\cosh(\sqrt{a-\sqrt{b}}/kT)}, \tag{18}$$

where a and b were given in Eq. (11). Before we start to discuss the results of numerical calculations at different temperatures and magnetic fields let us consider the less complicated case of $T=0$. The simplified formula for S_0 takes the form

$$\overline{S_0}=\frac{h_0}{2\sqrt{a+\sqrt{b}}}\left(1+\frac{4A^2\overline{\sigma_z^2}+\Delta^2\gamma^2}{2\sqrt{b}}\right). \tag{19}$$

From this formula it can be seen that the presence of the electron-electron correlations $(A\neq 0)$ caused by virtual phonon exchange leads to an additional nonlinear dependence of the magnetic moment upon the field because $\overline{\sigma_z}$ is a complicated function upon H. As a consequence of that, an anomalous ''knee'' appears in the $M(H)$ dependence. It is easy to see that if $A=0$ the regular saturation of a magnetic moment of a paramagnetic material under high fields takes place. In this situation of no structural phase transitions, the magnetic moment is described by

$$\overline{S_0}=\frac{h_0(1+\Delta\gamma/\sqrt{\Delta^2\gamma^2+2h_0^2})}{2\sqrt{h_0^2/2+(\Delta^2\gamma^2/2)(1+\sqrt{1+2h_0^2/\Delta^2\gamma^2})}}, \tag{20}$$

from which we obtain the result that at very big magnetic fields $(h_0 \gg \Delta)\overline{S_0}\rightarrow\sqrt{2}/2$. As is seen from Figs. 1, 2, 5, and 6 the anomaly connected with the structural phase transition is quite small and could be more easily observed at the measurements of the magnetic susceptibility that was calculated from Eq. (18). As it is shown in Figs. 1, 2, 5, and 6, a small but sharp jump at $T=T_c$ and $H_0=H_{\mathrm{crit}}$ appears.

ELASTIC PROPERTIES

The elastic susceptibility is the reaction function connected with the order parameter at the structural phase transitions. Since the field-induced structural transitions under consideration are of ferroelastic type the elastic susceptibility is expected to diverge at $T=T_c$ and $H=H_{\mathrm{crit}}$. The corresponding modulus of elasticity C is supposed to go to zero $[C(T=T_c)=0]$. At the structural transitions from tetragonal to orthorhombic phase, induced by the magnetic field, the soft modulus of elasticity is $C=C_{66}$. This modulus determines the velocity of the transverse mode propagating along the [100] direction with the polarization vector parallel to [010] direction. As it is known from the cooperative Jahn-Teller effect theory, the measurements of the the temperature and field dependences provide a lot of information about the system under investigation and in part allow the determination of the electron-strain interaction constant. The last is especially important as this interaction is the main contribution to the electron-electron interaction responsible for the phase transition in the TmPO_4 and $\mathrm{Tb}_x\mathrm{Y}_{1-z}\mathrm{VO}_4$ crystals.

The modulus of elasticity can be calculated if in Hamiltonian (2) the applied uniaxial stress P of $B_{2g}(D_{4h})$ symmetry is included. The corresponding term of the Hamiltonian is

$$H_P=-\frac{g_0}{\sqrt{C_0\Omega N}}\,P\sum_m \sigma_z^m. \tag{21}$$

The equation for the order parameter has the same form, with the only difference being that all $A\overline{\sigma_z}$ are replaced with

$$A\overline{\sigma_z}+\frac{g_0P}{\sqrt{C_0\Omega N}}.$$

Taking into account that the modulus of elasticity is defined as

$$C^{-1}=\left(\frac{\partial U}{\partial P}\right)_{P=0} \tag{22}$$

and

$$U=g_0\sqrt{\frac{N}{C_0\Omega}}\,\overline{\sigma_z}, \tag{23}$$

the formula for $C=C(H,T)$ can be determined. For simplicity the formula for $T=0$ only will be shown

$$\frac{C}{C_0}=\frac{(1-A/\sqrt{a+\sqrt{b}})F_0}{[1-(A-g_0^2)/\sqrt{a+\sqrt{b}}]F_0}, \tag{24}$$

where

$$F_0=1+\frac{h_0^2}{\sqrt{b}}-\overline{\sigma_z^2}\left[1-2\,\frac{a+\sqrt{b}}{\sqrt{b^3}}\,\frac{h_0^4}{(1+h_0^2/\sqrt{b})^2}\right]. \tag{25}$$

The results of the calculations of the temperature and the magnetic-field dependences for the modulus of elasticity are shown in Figs. 3, 4, 7, and 8. The modulus of elasticity dips to zero at the critical temperatures and critical values of the external magnetic field. If the reentrant phase transitions take place the modulus of elasticity becomes zero, twice remaining small enough but not zero at $T_{c1}<T<T_{c2}$.

CONCLUSIONS

In the framework of the cooperative Jahn-Teller effect the microscopic theory of the magnetic-field-induced structural phase transitions is developed. The coupling between macroscopic and microscopic parameters is found. The experiments on giant magnetostriction[12] and on Raman scattering of light confirm the theoretical prediction of the phenomenon.[13] Different magnetic, magnetoacoustic, and elastic properties are investigated and a series of anomalies connected to the phase transition are predicted. These results are waiting for further experimental verification.

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