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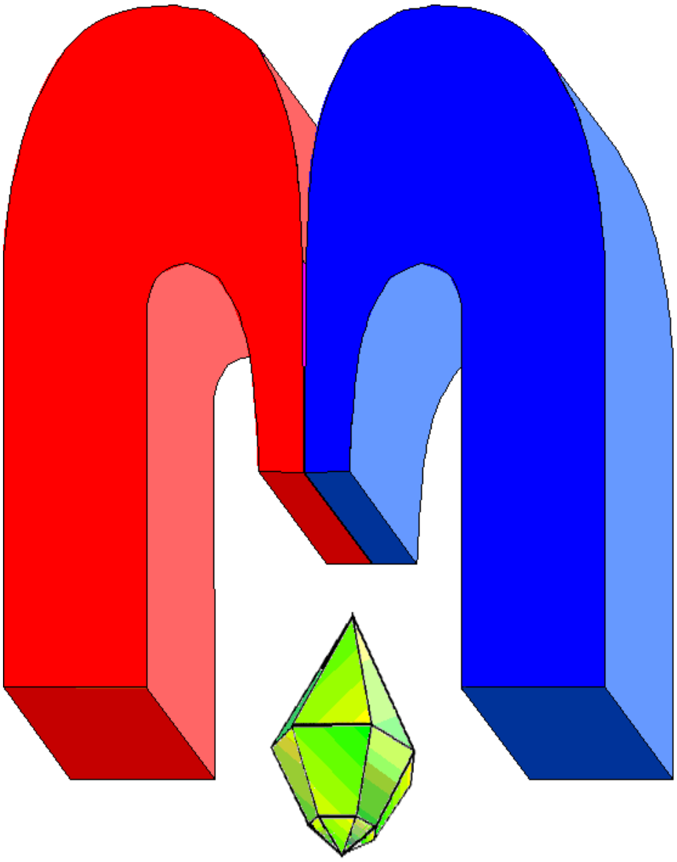

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[*] In Kazan University the Electron Paramagnetic Resonance (EPR) was discovered by Zavoisky E.K. in 1944.

Simulations of equilibrium magnetic and magnetoelastic properties of non-conducting rare-earth compounds[†]

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The Hamiltonian of the magnetic subsystem containing rare-earth ions involves energies of the localized 4f-electrons in free ions, energies of interactions of the 4f-electrons with the static crystal field in the perfect crystal lattice as well as in the homogeneously deformed lattice, interactions with the external magnetic field and lattice vibrations (electron-phonon interaction), magnetic dipolar and exchange interactions between the ions. This Hamiltonian is used in calculations of different measurable physical parameters versus temperature and the magnetic field strength and direction (energy levels of rare earth ions, the magnetization, magnetic dc- and ac-susceptibilities, elastic constants, lattice deformations)

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Keywords: crystalline electric field parameters, magnetostriction, magnetoelastic interaction, electron-phonon interaction

1. Introduction

The construction of the energy spectrum of the rare earth ion in the crystalline electric field is of actual interest for scientists engaged in the study of solid crystalline substances containing rare-earth ions [1, 2]. Based on the obtained spectrum one can describe the field, angle and temperature dependences of magnetization and susceptibility, the dependence of the energy levels on the external magnetic field and temperature, the magnetic field and temperature dependences of the elastic constants, deformations of unit cell [3]. The most convenient in this case, is a software package MATLAB. The basic principles of such calculations are presented in this article and the results are shown for the case of rare earth tetrafluorides [4-8].

Double fluorides of rare earths are the subject of intensive research over the past three decades, and the study of their magnetic properties remains relevant for the further development of the theory of magnetoelastic effects in magnetic materials containing rare-earth ions [9-14]. The calculation results are used to interpret the data of the magnetic properties studies of single crystals of the rare earths double fluorides in the frame of magnetoelastic and electron-phonon interaction models [4-8].

The unit cell of $LiLnF_4$ contains two magnetically equivalent lanthanide Ln^{3+} ions at sites with the S_4 point symmetry. The crystal lattice of the compounds $LiLnF_4$ is shown in Figure 1 [9].

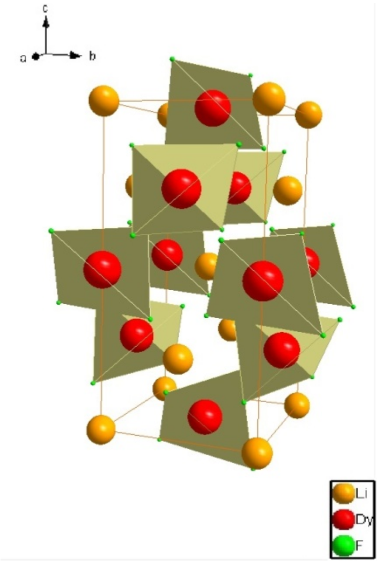

Figure 1. The crystal lattice of the $LiLnF_4$ compounds.

Magnetic properties of $LiLnF_4$ are shown in Table 1. $LiTbF_4$ and $LiHoF_4$ are dipolar Ising-like ferromagnets with magnetic moments of the Tb^{3+} and Ho^{3+} ions along the crystallographic c-axis and Curie temperatures $T_c = 2.885$ K and 1.53 K, respectively [9]. $LiDyF_4$ is antiferromagnet of easy-plane type with magnetic moments of the Dy^{3+} ions normal to the crystal

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[†] This paper is prepared on base of invited lecture at XIX International Youth Scientific School "Actual problems of magnetic resonance and its application", Kazan, 24 – 28 October 2016 and it is published after additional MRSej reviewing.

Table 1. The $LiLnF_4$ compounds magnetic properties.

$LiTmF_4$ $4f^{12}$	$LiTbF_4$ $4f^{8}$	$LiHoF_4$ $4f^{10}$	$LiDyF_4$ $4f^{9}$
Van-Vleck paramagnet	Ising-like dipole ferromagnet	Ising-like dipole ferromagnet	Dipole antiferromagnet
-	$T_c = 2.89$ K	$T_c = 1.53$ K	$T_N = 0.62$ K

symmetry axis, and transition temperatures $T_N = 0.62$ K [9]. The $LiTmF_4$ is Van-Vleck paramagnet [9]. Magnetic dipole-dipole interactions play the dominant role in spontaneous low-temperature ordering of magnetic moments of Ln^{3+} ions in these compounds. Quantum phase transitions driven by transverse magnetic fields were observed in $LiHoF_4$ at temperatures below T_c [15]. $LiTmF_4$ exhibit a giant forced magnetostriction at liquid helium temperatures [16].

2. The theoretical background

The Hamiltonian of magnetic system of rare-earth ions can be written by taking into account an interaction with crystallographic lattice and free surface, the ion energy in crystal field, the electron Zeeman energy, interaction of rare-earth ion with homogeneous macro- and microdeformations, magnetic dipolar and exchange interactions between the ions and electron-phonon energy [9].

The Hamiltonian of magnetic system of rare-earth ions which take an interaction with a crystallographic lattice and a free surface into account can be written as:

$$H = \sum_{Ls} H_{L,s} + H_{lat} + \sum_{Ls}\sum_{\mathbf{q}j}\sum_{pk}\frac{1}{\sqrt{N}} B_p^k(s,\mathbf{q}j)\exp(i\mathbf{q}\mathbf{R}_{Ls})O_p^k(Ls)Q(\mathbf{q}j). \tag{1}$$

Here $H_{L,s}$ is the Hamiltonian of rare earth ion with the radius-vectror $\mathbf{R}_{Ls}$ from s-sublattice ($s = 1, 2$) in cell L in static crystal field, H_{lat} is energy of crystal lattice in harmonic approximation with normal coordinates $\mathbf{Q}(\mathbf{q}j)$ ($\mathbf{q}$ is wave phonon vector with frequency ω_{qi}, j is the number of oscillation spectrum branch), the last part in (1) presents electron-phonon energy in linear approximation on ions displacements from equilibrium condition, N is cell number, $O_p{}^k(L, S)$ is linear combination of spherical tensor operators [9], in force in space of electron states of rare earth ion in L_s, $B^k{}_p(s, \mathbf{q}j)$ are interaction parameters, determined by derivatives of corresponding crystal field parameters on ions [8].

Considering the second order corrections to rare-earth ion's energy by electron-phonon interaction at low temperature ($k_BT << \hbar\omega$, k_B is Bolzman constant, ω_0 is limiting phonon frequency) and taking into account only mixing electrons with difference energies $\Delta << \hbar\omega_0$, we can write the effective Hamiltonian of interaction between Ln^{3+} ions [17]

$$\Delta H = -\frac{1}{2}\sum_{LL'ss'}(1-\delta_{LL'}\delta_{ss'})\sum_{pp'kk'}\Phi_{pp'}^{kk'}(ss',\mathbf{R}_{LL'}^{ss'})O_p^k(Ls)O_{p'}^{k'}(L's'), \tag{2}$$

where $\mathbf{R}_{LL'}^{ss'} = \mathbf{R}_{Ls} - \mathbf{R}_{L's'}$, and

$$\Phi_{pp'}^{kk'}(ss',\mathbf{R}_{LL'}^{ss'}) = \frac{1}{N}\sum_{\mathbf{q}j}\omega_{\mathbf{q}j}^{-2}B_p^k(s,\mathbf{q}j)B_{p'}^{k'}(s',-\mathbf{q}j)\exp(i\mathbf{q}\mathbf{R}_{LL'}^{ss'}). \tag{3}$$

Double-particle interactions can be considered in self-consistent field approximation, with neglecting the second order terms on operator's deviations $O_p^k(Ls)$ from their average values $< O_p^k(Ls) > = < O_p^k >$ (the last equation appears if all magnetic ions are equivalent, particularly, for Ln^{3+} ions in $LiLnF_4$).

The free energy of elastic distorted single crystal in presence of an applied magnetic field $\mathbf{B}$ (on the elementary cell with volume v) can be written in the following form:

$$F=\frac{v}{2}[\mathbf{eC'e}+2\sum_{s}\mathbf{eb}(r)\mathbf{w}(r)+\sum_{s\,s'}\mathbf{w}(r)\mathbf{a}(r,r')\mathbf{w}(r')]+\frac{n}{2}\sum_{pkp'k'}\left\langle O_p^k\right\rangle\boldsymbol{\lambda}_{pp'}^{kk'}\left\langle O_{p'}^{k'}\right\rangle+\Delta F,$$

$$\Delta F=-\sum_{s}k_BT\ln\mathrm{Tr}\exp(-H_{eff,s}/k_BT), \qquad (4)$$

where **C**' is tensor of "probe" elastic constants, **e** is the deformation tensor, **w**(r) is vector of the sublattice displacement r, **b**(r) is the relation's constants tensor of macro- and microdeformations, $a_{\alpha\beta}(r,r')$ is the dynamic matrix of the lattice at the Brillouin zone centre, $\lambda_{pp'}^{kk'}$ is the matrix of the relation's constants through phonon field, n is number equivalent magnetic sublattices ($n=2$ for LiLnF$_4$ single crystal), H$_{\mathrm{eff,s}}$ is effective single-ion Hamiltonian, defined below:

$$H_{eff}=H^{(0)}+H^{(P)}, \qquad (5)$$

$$H^{(0)}=H_0+H_{cf}+H_Z, \qquad (6)$$

$$H^{(P)}=\sum_{\alpha\beta}V_{\alpha\beta}e_{\alpha\beta}+\sum_{\alpha,s}V_\alpha(s)w_\alpha(s)-\sum_{pkp'k'}\lambda_{pp'}^{kk'}<O_p^k>O_{p'}^{k'}. \qquad (7)$$

The first part in (6) is the Hamiltonian of free ion H$_0$, the second term is the ion energy in crystal field, the third term is the electron Zeeman energy $H_Z=\mu_B\mathbf{B}(\mathbf{L}+2\mathbf{S})$; here μ_{B} is the Bohr magneton. First and second terms in (7) define linear interaction of rare-earth ion with homogeneous macro- and microdeformations, correspondingly. Electronic operators $V_{\alpha\beta}$ and $V_{\alpha(s)}$ can be presented as linear combinations of spherical tensor operators:

$$V_{\alpha\beta}=\sum_{pk}B_{p,\alpha\beta}^kO_p^k,\ V_\alpha(r)=\sum_{pk}D_{p,\alpha}^k(r)O_p^k. \qquad (8)$$

Taking into account translational lattice symmetry one can find from equations (2) and (3) the following equation for λ matrix elements in last term in (7):

$$\lambda_{pp'}^{kk'}=\frac{1}{n}\sum_{ss'}\left[\sum_{j_o}\frac{B_p^k(s,0j_o)B_{p'}^{k'}(s',0j_o)}{\omega_{\mathbf{0}j_o}^2}-\frac{\delta_{ss'}}{N}\sum_{\mathbf{q}j}\frac{B_p^k(s,\mathbf{q}j)B_{p'}^{k'}(s',-\mathbf{q}j)}{\omega_{\mathbf{q}j}^2}\right], \qquad (9)$$

where the first term includes only optical branches of oscillation spectrum. The single ion contribution to the free energy (see equation (4)) can be written with accuracy up to second order terms of lattice deformations lattice and deviations of average values operators O_p^k from corresponding equilibrium values in absence of magnetic field (for the simplicity equations below $<O_p^k>_{\mathbf{B}=0}=0$ is supposed). Considering operator (7) as perturbation one can rewrite $H^{(P)}=\sum_{pk}A_p^kO_p^k=A:O$, and obtain

$$\Delta F=n[F_0(\mathbf{B})+<H^{(P)}>_0+\frac{1}{2}A:q:A], \qquad (10)$$

where $F_0(\mathbf{B})$ is the free ion energy with Hamiltonian $H^{(0)}$, symbol $<...>_0$ means averaging with equilibrium density matrix $\rho=\exp(-H^{(0)}/k_BT)/\mathrm{Tr}(\exp(-H^{(0)}/k_BT))$. The matrix elements q equal:

$$\begin{aligned}q_{pp'}^{kk'}=\frac{1}{k_BT}[<O_p^k>_0<O_{p'}^{k'}>_0-\sum_i\langle\psi_i|\rho O_p^k|\psi_i\rangle\langle\psi_i|O_{p'}^{k'}|\psi_i\rangle]\\+\sum_{i,j\neq i}(\varepsilon_i-\varepsilon_j)^{-1}[\langle\psi_i|\rho O_p^k|\psi_j\rangle\langle\psi_j|O_{p'}^{k'}|\psi_i\rangle+\langle\psi_i|\rho O_{p'}^{k'}|\psi_j\rangle\langle\psi_j|O_p^k|\psi_i\rangle].\end{aligned} \qquad (11)$$

Here ε_i and ψ_i are eigenvalues and eigenfunctions of $H^{(0)}$ operator.

Taking into account thermodynamic equilibrium conditions $\partial F/\partial<O_p^k>=0$, $\partial F/\partial w_\alpha(r)=0$ and symbol of convolution on indexes *p* and *k*, introduced above, one can write the free crystal energy as

$$\begin{aligned} F = \frac{v}{2}\mathbf{eCe} + nF_0 - \frac{n}{2} < O >_0 : [\lambda : (1 + q : \lambda)^{-1} + \frac{n}{v}\sum_{rr'} \hat{\mathbf{D}}(r)\hat{\mathbf{a}}^{-1}(r,r')\hat{\mathbf{D}}(r')] :< O >_0 \\ + n < O >_0 : (1 + \lambda : q)^{-1} : [\mathbf{B} - \sum_{rr'} \hat{\mathbf{b}}(r)\hat{\mathbf{a}}^{-1}(r,r')\mathbf{D}(r')]\mathbf{e}, \end{aligned} \tag{12}$$

where $\hat{D}_\alpha(r) = (1 + \lambda : q)^{-1} : D_\alpha(r)$, $\mathbf{C} = \hat{\mathbf{C}}' - \sum_{rr'} \hat{\mathbf{b}}(r)\hat{\mathbf{a}}^{-1}(r,r')\hat{\mathbf{b}}(r')$ is the elastic constants tensor. The definitions of renormalized values through electron-deformation and electron-phonon interactions:

$$\hat{a}_{\alpha\beta}(r,r') = a_{\alpha\beta}(r,r') + \frac{n}{v} D_\alpha(r) : q : (1 + \lambda : q)^{-1} : D_\beta(r'), \tag{13}$$

$$\hat{b}_{\alpha\beta,\gamma}(r) = b_{\alpha\beta,\gamma}(r) + \frac{n}{v} B_{\alpha\beta} : q : (1 + \lambda : q)^{-1} : D_\gamma(r), \tag{14}$$

$$\hat{C}'_{\alpha\beta\gamma\delta} = C'_{\alpha\beta\gamma\delta} + \frac{n}{v} B_{\alpha\beta} : q : (1 + \lambda : q)^{-1} : B_{\gamma\delta}. \tag{15}$$

It should be noted, that temperature and magnetic field dependences of elastic constants can be written in following form with accuracy up to second order components of electron-deformation interaction's parameters:

$$C_{\alpha\beta\gamma\delta}(T,\mathbf{B}) = C_{\alpha\beta\gamma\delta}(T = 0, \mathbf{B} = 0) + \frac{n}{v} \hat{B}_{\alpha\beta} : q : (1 + \lambda : q)^{-1} : \hat{B}_{\gamma\delta}, \tag{16}$$

where renormalization relation's constants of macro- and micro-deformations equal:

$$\hat{B}^k_{p,\alpha\beta} = B^k_{p,\alpha\beta} - \sum_{rr'\gamma\delta} b_{\alpha\beta,\gamma}(r) a^{-1}_{\gamma\delta}(r,r') D^k_{p,\delta}(r'). \tag{17}$$

The relative change of single crystal size induced by magnetic field in the direction defined by unit vector with directional cosines n_α equals $\Delta l / l = \sum_{\alpha\beta} n_\alpha n_\beta e_{\alpha\beta}$, where components of deformation tensor define from minimum free energy condition (12):

$$\mathbf{e}(\mathbf{B}) = -\frac{n}{v}[\mathbf{SB}_{eff} :< O >_0\big|_{\mathbf{B}} - \mathbf{SB}_{eff} :< O >_0\big|_{\mathbf{B}=0}], \tag{18}$$

here ${B_{eff}}^k_{p,\alpha\beta} = \sum_{p'k'} [(1 + \lambda : q)^{-1}]^{kk'}_{pp'} : \hat{B}^{k'}_{p',\alpha\beta}$, $\mathbf{S} = \mathbf{C}^{-1}$ is the compliance tensor.

Ion's energy levels and their magnetic moments in external magnetic field are determined by effective Hamiltonian, introduced above, where perturbation operator is:

$$H^{(P)} = \{\mathbf{B}_{eff}\mathbf{e} - < O >_0 : [\frac{n}{v}\sum_{rr'} \hat{\mathbf{D}}(r)\hat{\mathbf{a}}^{-1}(r,r')\hat{\mathbf{D}}(r') + \lambda : (1 + q : \lambda)^{-1}]\} : O. \tag{19}$$

Equations defined above for elastic constants, induced by magnetic field and for effective Hamiltonian of paramagnetic ion are used for calculation of single crystal $LiLnF_4$ parameters.

3. Calculation and programming in the simplified case

At the first step the Hamiltonian of a single Ln^{3+} ion can be written in the following form:

$$H = H_0 + H_{cf} + \sum_{\alpha\beta} V_{\alpha\beta} e_{\alpha\beta} + \sum_{\alpha,s} V_\alpha(s) w_\alpha(s) + \sum_j [\mu_B(\mathbf{B} + \tilde{Q}\mathbf{M})(\mathbf{l}_j + 2\mathbf{s}_j) - \sum_{pkp'k'} \lambda^{kk'}_{pp'} < O^k_p > O^{k'}_{p'}]. \tag{20}$$

Here, the first term is the free ion energy, the second term is the crystal field Hamiltonian:

$$H_{cf} = B^0_2 O^0_2 + B^0_4 O^0_4 + B^4_4 O^4_4 + B^{-4}_4 O^{-4}_4 + B^0_6 O^0_6 + B^4_6 O^4_6 + B^{-4}_6 O^{-4}_6, \tag{21}$$

determined in the crystallographic system of coordinates by the set of seven crystal field parameters B_p^k (O_p^k are the Stevens operators). The third and fourth terms correspond to linear interactions of rare-earth ions with the homogeneous macro- and micro-deformations, respectively, where **e** is the deformation tensor, and **w**(s) is the vector of the s-sublattice displacement. The electronic operators V' and V''(s) similar to the crystal field energy can be presented through the linear combinations of Stevens operators with the parameters which have been calculated earlier in the framework of the exchange charge model (see [18]).

The fifth term in (20) is the electronic Zeeman energy where μ_B is the Bohr magneton, $\mathbf{l}_j$ and $\mathbf{s}_j$ are operators of orbital and spin moments, **M** is the equilibrium magnetization, the tensor **Q** defines magnetic dipole-dipole interactions between the rare-earth ions, and the sum is taken over 4f electrons. The last term corresponds to the energy of interaction between paramagnetic ions via the phonon field, parameters $\lambda_{pp'}^{kk'}$ were calculated by making use of the characteristics of the lattice dynamics of the $\mathrm{LiLnF_4}$ crystal lattices.

The crystal free energy (per unit cell) is written as:

$$F = \frac{v}{2}(\mathbf{eC'e} + \mathbf{waw} + 2\mathbf{ebw}) + <\mathbf{O}> \boldsymbol{\lambda} <\mathbf{O}> - v\mathbf{MB} - nk_B T \ln \mathrm{Tr} \exp(-H / k_B T), \tag{22}$$

where v is the volume of the unit cell, k_B is the Boltzman constant, $\mathbf{C} = \mathbf{C}' - \mathbf{ba}^{-1}\mathbf{b}$ is the tensor of elastic constants, **a** is the dynamic matrix of the lattice at the Brillouin zone centre, the tensor **b** determines linear coupling between macro- and microdeformations, $n = 2$ is the number of rare-earth ions in the unit cell, and angular brackets <…> mean the thermal averaging. From the equilibrium conditions for the coupled paramagnetic ions and the elastic crystal lattice

$$\partial F / \partial < O_p^k > = \partial F / \partial e_{\alpha\beta} = \partial F / \partial w_\alpha(s) = \partial F / \partial B_\alpha = 0\,, \tag{23}$$

self-consistent equations for the magnetization vector and the deformation tensor components can be obtained. In particular, the lattice macro-deformation induced by the external magnetic field is determined by the expression:

$$\mathbf{e}(\mathbf{B}) = -\frac{n}{v}\mathbf{S}[\langle \mathbf{V} \rangle_B - \langle \mathbf{V} \rangle_0]\,, \tag{24}$$

and the sublattice displacements, which define the internal magnetostriction, equal

$$\mathbf{w}(\mathbf{B}) = -\frac{n}{v}\mathbf{a}^{-1}[\langle \mathbf{V}'' \rangle_B - \langle \mathbf{V}'' \rangle_0] - \mathbf{a}^{-1}\mathbf{be}(\mathbf{B})\,. \tag{25}$$

Here **S** is the compliance tensor of the lattice, and angular brackets $<...>_B$, $<...>_0$ indicate thermal averages for $B \neq 0$ and $B = 0$, respectively. Operators **V** in the expression (24) equal to operators **V**′ renormalized due to linear coupling of macro- and micro-deformations ($\mathbf{V} = \mathbf{V}' - \mathbf{ba}^{-1}\mathbf{V}''$).

The system of equations (23) was solved using the method of successive approximations at fixed values of the temperature and the external magnetic field. The procedure involved the following steps: first, the matrix of the Hamiltonian (20) with **M** = 0, **e** = 0, **w** = 0 is diagonalized, and the macro- and micro-deformations (**e**(**B**) and **w**(**B**)), and the magnetization **M** are calculated. At the next step, the obtained values of **M**, **e**, **w** are substituted into the Hamiltonian and the calculations are repeated. Considering the power series expansion of the free energy in deformation parameters up to second order corrections to the elastic constants depending on the magnetic field and temperature can be found. At the last step, the obtained values of **M**, **e**, **w** and **C**(**B**) are substituted into the Hamiltonian and the values of **M** are calculated [4-8].

The simple example of calculation's program is presented here. At the first step Stevens matrix operators should be entered to the code (on MATLAB software):

```
O20=zeros(16,16);
O20(1,1)=35;
O20(2,2)=21;
O20(3,3)=9;
O20(4,4)=-1;
O20(5,5)=-9;
O20(6,6)=-15;
O20(7,7)=-19;
O20(8,8)=-21;
for i=9:16
  O20(i,i)=O20(17-i,17-i);
end;
```

In the next step the matrix elements of angular momentum operator $J = 15/2$ (as an example) is input:

```
Jz=zeros(16,16);
for i=1:16
  Jz(i,i)=17/2-i;
end;
```

The Hamiltonian of the crystal field has a following form in code:

```
H0=B20*O20+B40*O40+B44*O44+B44m*O44m+B60*O60+B64*O64+B64m*O64m;
```

The strength of external magnetic field (in Oe) is input:

```
H1=10000;
```

The Zeeman Hamiltonian (magnetic field is directed along x- or z-axes):

```
HZ=g0*m*H1*Jx;
HZ=g0*m*H1*Jz;
Hfull=H0+HZ;
```

The diagonalization of the total Hamiltonian define eigenstates and eigenfunction of presented Hamiltonian:

```
[V, D]=eig(Hfull);
d=eig(Hfull);
```

4. Discussion and result

A large array of experimental data can be self-consistently described using this calculation method. Each compound has its own set of the crystal field parameters, the electron-deformation interaction parameters, elastic constants and constants of the electron-phonon interaction. Some results are presented in the following figures (2-9).

The experimental dependence of the elastic constants of the temperature is well described in the model and the energy of the deformed lattice can be estimated. The results are shown in Figure 2 [8].

The field and temperature dependences of the energy levels splitting are well described in the framework of this approach. The example of the results is shown in Figure 3.

The relative change in size of the crystal along the direction of the field is equal to:

$$\Delta l / l = e(A_g^2) + \frac{1}{2}\cos 2\varphi e(B_g^1) + \sin 2\varphi e(B_g^2)\,. \tag{26}$$

The obtained deformation tensor components values are satisfactory agree with measurements of the longitudinal magnetostriction in $LiTmF_4$ single crystal (Figure 3) [8], $LiDyF_4$ single crystal (Figure 4) [7].

The results of calculations predict that the magnetostriction strongly anisotropic and reaches giant values of the order of 10^{-3} in a magnetic field about 1 T at $T = 4.2$ K (Figure 5).

The results of calculation and comparison with experimental data angle (Figure 6), temperature and field dependences (Figure 7a,b) of the magnetization for various compounds are shown below.

The described method of calculations allows to select and adjust the parameters of the crystal field. An example is shown in Figure 8 for the single crystal $LiTbF_4$ [4, 5].

The calculations show the strong anisotropy of the magnetization as a function of the direction of the applied magnetic field relative to the crystal lattice axes. The results of calculation are shown in Figure 9 [7].

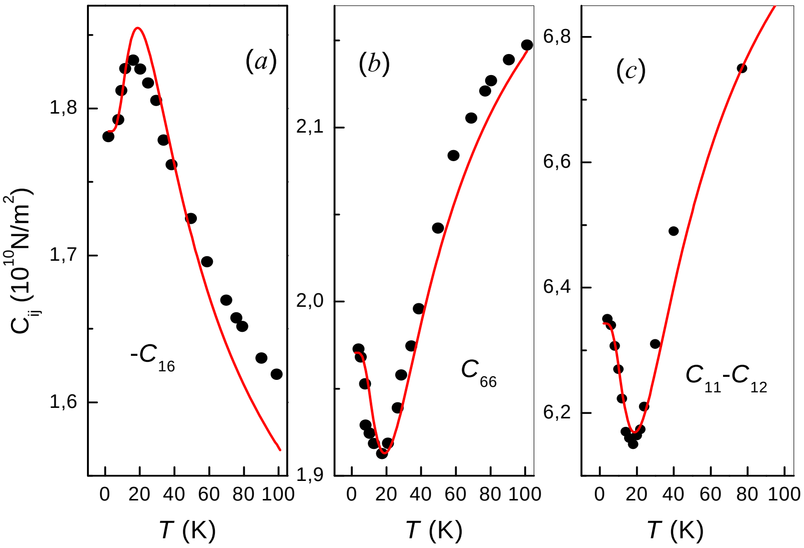

Figure 2. Measured [19] (symbols) and calculated [8] (curves) the temperature dependence of the elastic constants C_{16} (*a*), C_{66} (*b*) and $C_{11} - C_{12}$ (*c*) $LiTmF_4$ single crystal.

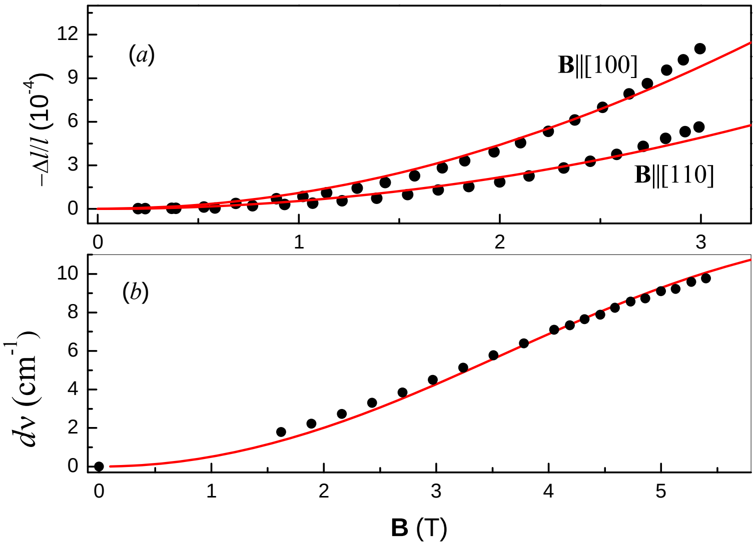

Figure 3. Field dependence at 4.2 K (*a*) of the longitudinal magnetostriction in an external magnetic field **B** and (*b*) the splitting of the doublet $\Gamma_{34}(1)$ in a magnetic field, oriented in the basal plane of a single crystal $LiTmF_4$ angle $\varphi = 10°$ to the axis *a*. The calculation results are represented by lines, symbols correspond to the experimental data [8].

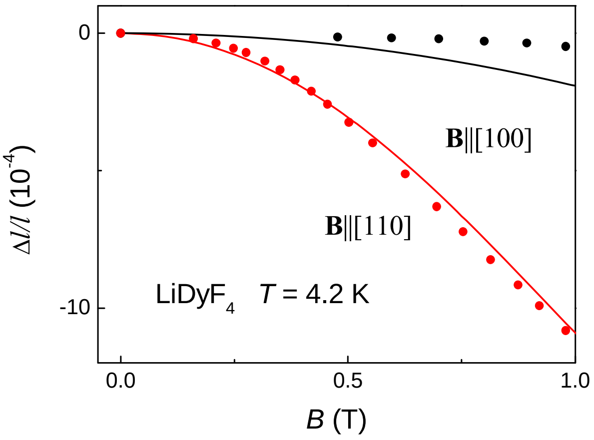

Figure 4. Field dependence of the magnetostriction in the two directions of the applied magnetic field in $LiDyF_4$ single crystal at $T = 4.2$ K. The calculation results are represented by lines, symbols correspond to the experimental data [7].

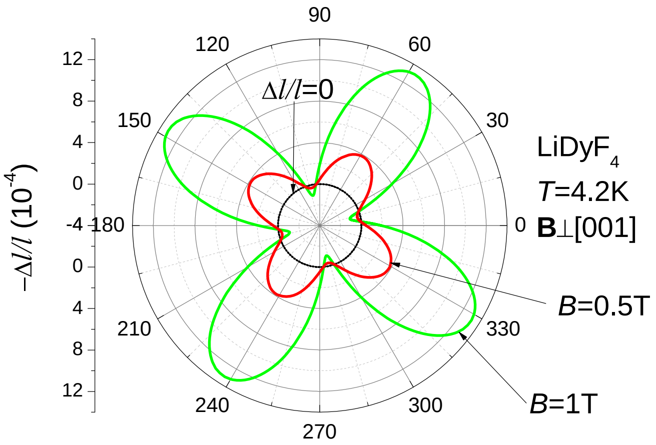

Figure 5. The calculated angular dependence of the magnetostriction in a magnetic field $B = 1$ T (curve 1) and 0.5 T (curve 2), $T = 4.2$ K.

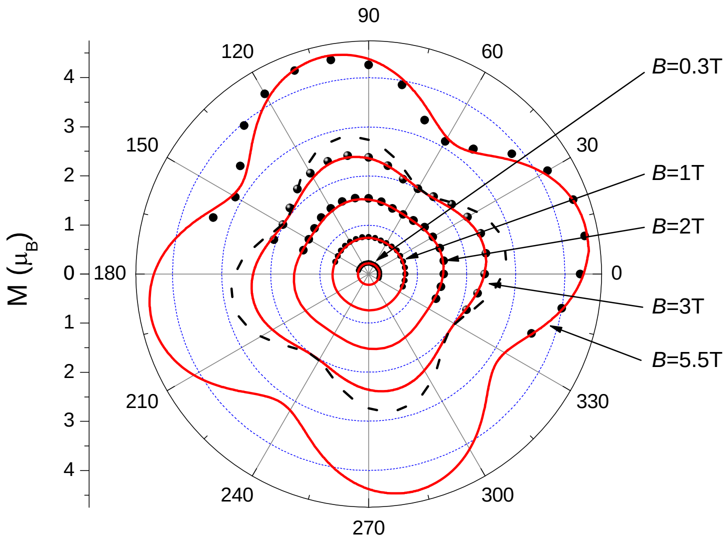

Figure 6. Measured (symbols) [3] and calculated [8] $LiTmF_4$ single crystal's magnetization angular dependences in the external magnetic field **B** in the basal plane of the lattice, $T = 4.2$ K.

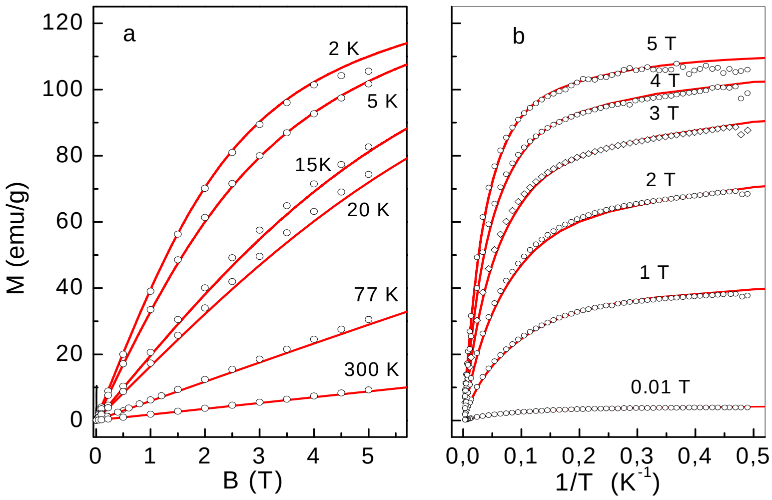

Figure 7. Field (a) and temperature (b) dependences of the magnetization along the axis of a single crystal of $LiHoF_4$. Solid lines are theoretical results, symbols are experimental data [6].

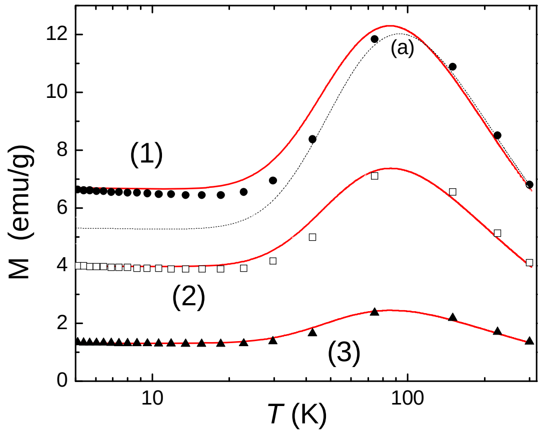

Figure 8. Measured (symbols) and calculated the temperature dependence of magnetization $LiTbF_4$ single crystal in a magnetic field $\mathbf{B} \perp$ c; $B = 5$ T (1), 3 T (2), 1 T (3) (dotted line shows calculation with a set of crystal field parameters from the literature) [4].

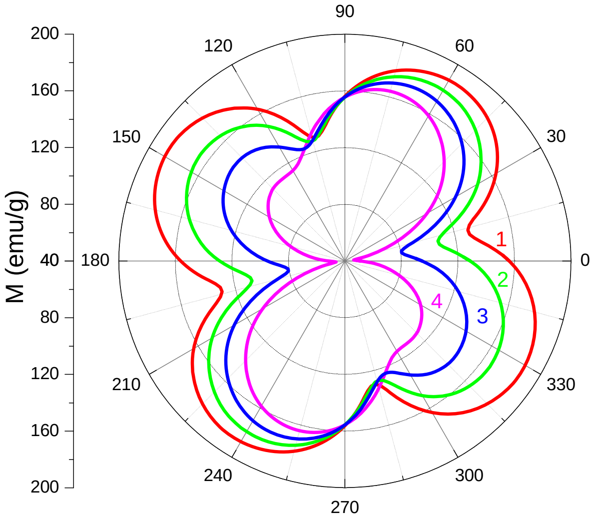

Figure 9. The calculated angular dependence $LiDyF_4$ single crystal magnetization in an external magnetic field in different planes ($B = 2$ T): curve 1 shows calculation results at $\theta = 0$, $\alpha = 0$; curve 2 shows calculation results at $\theta = 5°$, $\alpha = 30°$; curve 3 shows calculation results at $\theta = 5°$, $\alpha = 45°$; curve 4 shows calculation results at $\theta = 5°$, $\alpha = 60°$ [7].

5. Conclusion

The presented method makes it possible to solve the following tasks:

1) The determination of the parameters of the crystal field.
2) The calculation of the magnetoelastic interaction contribution to the magnetization.
3) The calculation of the contribution of the interaction between the rare-earth ions via phonon field.
4) The determination of the field, temperature and angular dependences of the magnetization, magnetostriction and the energy levels spectrum of the rare earth ion.

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