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Intermetallics

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Application of the exchange-striction model for the calculation of the FeRh alloys magnetic properties



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ARTICLE INFO

Keywords: FeRh alloys First order phase transition Exchange striction

ABSTRACT

Application of the exchange-striction model for the calculation of the magnetic properties of antiferro (AFM) and ferromagnetic (FM) phases of the iron-rhodium alloy is proposed. The following properties of the antiferromagnetic phase have been calculated and compared with the experimental data: the temperature dependences of the sublattice magnetization, the relative change in volume and entropy, and the pressure dependence of the Néel temperature. For the ferromagnetic phase, the temperature dependence of the magnetization, the dependence of the volume and entropy on temperature, and the dependence of the Curie temperature on pressure were calculated. A satisfactory agreement between the results of calculations and experiment has been obtained. The reasons for the AFM-FM phase transition in the iron-rhodium alloy are discussed.

1. Introduction

With increasing temperature, the ordered $Fe_{50}Rh_{50}$ alloy undergoes a first-order phase transition from the antiferromagnetic (AFM) to the ferromagnetic (FM) phase [1,2]. This transition occurs at a temperature T_N in the temperature range from RT to ~ 400 K. The transition temperature depends strongly on the specific composition and the presence of defects in the crystal structure [3,4]. The transition is accompanied by an increase in volume of about 1%, while the crystal structure of B2 (bcc, CsCl type) does not change [5–7]. Moreover, some theoretical calculations show [8,9] that an orthorhombic structure in the AFM phase can be stable with the energy that is by several meV/atom less than the energy of the cubic B2 structure.

The maximal magnetocaloric effect (MCE) is observed in equiatomic FeRh alloys [4,10–13]. The values of the isothermal variation of the magnetic part of the entropy ΔS_M and the adiabatic temperature change ΔT reach values of up to $20 \text{ J kg}^{-1}\text{K}^{-1}$ and 13 K [10], in magnetic fields of 2 T, which is 3 times larger than the values of MCE in pure gadolinium. The value of MCE in FeRh alloys is 1.5 times greater than in other alloys with giant MCE known today: Gd₅Si_{4-x}Ge_x [14], La (Fe_xSi_{1-x}) [15], MnFeP (As, Ge) [16].

To clarify the reasons of the giant MCE in FeRh alloys, it is necessary to carry out complex experimental and theoretical studies of the firstorder magnetic phase transition. The theory of phase transitions of the first order was proposed by Kittel [17] (transitions with the inversion of the exchange interaction), and also by Bean and Rodbell [18].

Within the framework of these theories, it is shown that the cause of a first-order phase transition is a strong change in the exchange interactions and elastic energy with a change in the crystal lattice parameter. The model considering this mechanism of the magnetic phase transition is called the exchange-striction model and proposed by Bean and Rodbell [18]. In this paper, we consider the application of the exchange-striction model (ESM) [18] to explain the magnetic properties of the iron-rhodium compound.

2. Theoretical model

Due to the large values of magneto-volume effects (the dependence of the volume on the magnitude of the magnetization) and the strong dependence of the Néel and Curie temperatures on pressure in Fe–Rh alloys [7,19] it is possible to develop the ESM of a ferromagnet taking into account the dependence of Curie temperature on the volume

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https://doi.org/10.1016/j.intermet.2019.02.015

Received 24 June 2018; Received in revised form 18 February 2019; Accepted 21 February 2019 0966-9795/ @ 2019 Elsevier Ltd. All rights reserved.





[20-23]. We used a version of the model developed earlier by the authors [24-26]. The main considerations for AFM and FM phases are presented in the subsections below.

2.1. Calculation of the AFM phase properties

According to the experimental data [27-29] and theoretical calculations [30,31], the magnetic moment of rhodium atoms in the AFM phase is zero. Therefore, it is assumed that the AFM ordering is formed by iron atoms. In the present work, FeRh is considered as an equiatomic ordered type CsCl alloy with a bcc lattice.

The nonequilibrium thermodynamic potential (model free energy) of the antiferromagnetic phase can be written as [24,32]:

$$F = \frac{1}{2}nJ_{11}s^{2}\sigma_{1}^{2} + \frac{1}{2}nJ_{22}s^{2}\sigma_{2}^{2} + nJ_{12}\sigma_{1}\sigma_{2}(\boldsymbol{e}_{1}\cdot\boldsymbol{e}_{2})s^{2} - nkT(\ln Z(y_{1}) + \ln Z(y_{2})) + \frac{1}{2}B\omega^{2} + P\omega + NkT\left(\ln(1 - e^{-\Theta/T}) - D\left(\frac{\Theta}{T}\right)\right).$$
(1)

In Eq. (1): the first four terms are the contributions of magnetic (exchange) interactions in the approximation of the theory of the effective (molecular) field [24,32], the terms 5 and 6 are the contributions of bulk elastic deformations in the presence of all-round compression [24,25]. The last term is the phonon contribution in the Debye-Grüneisen approximation. In addition, this term takes into account the thermal expansion of the lattice through the dependence of the Debye temperature on volume [25]. In the model used, only the exchange integral between the sublattices is assumed to depend on volume.

Also, in Eq. (1):

,

$$y_{1} = \left(\frac{s}{kT}\right) [2\mu(\boldsymbol{e}_{1}\cdot\boldsymbol{H}) + J_{11}s\sigma_{1} + J_{12}(\boldsymbol{e}_{1}\cdot\boldsymbol{e}_{2})s\sigma_{2}],$$

$$y_{2} = \left(\frac{s}{kT}\right) [2\mu(\boldsymbol{e}_{2}\cdot\boldsymbol{H}) + J_{22}s\sigma_{2} + J_{12}(\boldsymbol{e}_{1}\cdot\boldsymbol{e}_{2})s\sigma_{1}],$$

$$Z(y) = \frac{\sin h \left[(1 + (2s)^{-1})y\right]}{\sin h \left[((2s)^{-1})y\right]}, J_{11} = J_{22} = J_{11}^{0}, J_{12} = J_{12}^{0} + \gamma\omega, \Theta$$

$$= \Theta_{0} - \Gamma\omega\omega = \frac{\Delta V}{V},$$

 y_1 , y_2 - the ratio of the energy of the magnetic moment of an atom of type 1 or 2 in the effective (molecular) field acting on this atom from the surrounding atoms, to the thermal energy kT, s is a magnetic ion spin, μ is a Bohr magneton, H is the external magnetic field, e are the unit vectors of the direction of magnetization of AFM sublattices, σ_1 and σ_2 are the reduced magnetizations of the AFM sublattices, $J_{11} > 0$ and $J_{12} < 0$ are the intra-sublattice and inter-sublattice exchange integrals of the antiferromagnet, Θ is the Debye temperature, *B* is the modulus of all-round compression, *P* is pressure, γ and Γ are the constants of the magnetoelastic interaction and Grüneisen one, respectively, ω is the relative volume change (V), D (Θ/T) is the Debye function, n is the number of atoms per the unit volume for one sublattice of the antiferromagnet (half of the iron atoms per the unit volume of FeRh alloy), N is the total number of atoms per the unit volume of the alloy (N = 4n).

From the condition of the minimum of the thermodynamic potential (TP) Eq. (1) with respect to σ_1 , σ_2 and ω , the equilibrium state equations for the magnetizations of the sublattices and the relative change in volume ω can be obtained. When H = 0, $(\mathbf{e}_1 \cdot \mathbf{e}_2) = -1$, $\sigma_1 = \sigma_2 = \sigma$, $y_1 = y_2 = y$, these equations have the form:

$$\sigma = B_s(y) \tag{2}$$

$$\omega_{AF} = -ns^2 \sigma^2 \gamma B^{-1} + 3 \frac{NkT}{\Theta} \Gamma D\left(\frac{\Theta}{T}\right) B^{-1} - PB^{-1}$$
(3)

In Eq. (2) $B_s(y)$ is the Brillouin function for the spin s, and σ is the

reduced magnetization of the AFM sublattice, that is, the magnetizations of the sublattices $M_1 = -M_2 = 2\mu s\sigma n$, $y = \left[\frac{3kT_N^0 s\sigma}{s+1} - s^2\sigma\gamma\omega\right]/kT$, where $T_N^0 = s(s+1)(J_{11}^0 - J_{12}^0)/3k$ is the Néel temperature without taking into account the magnetoelastic interaction.

In Eq. (3) N is the total number of atoms per unit volume of the alloy. The first term in Eq. (3) (for $\gamma > 0$) is a negative spontaneous volume magnetostriction (SVM). The second term is the usual thermal expansion. The zero value of ω corresponds to the paramagnetic phase $(\sigma = 0)$ at T = 0 and P = 0. In the model used, a negative SVM is adopted, which is due to the fact that only in this case T_N increases with the application of pressure. A negative spontaneous volume magnetostriction indicates that the volume in the magnetically ordered (antiferromagnetic) state is smaller than in the paramagnetic state.

By the formulas Eqs. (1)–(3), the following dependences can be determined: the dependence of σ (T), the dependence of the Néel temperature on pressure, the temperature dependence of the magnetic part of the entropy, and ω (T). The equilibrium TP for given T, P, and H can be obtained using Eqs. (1)-(3). In this case, the numerical values of the parameters $J_{11}, J_{12}, \Theta, \Gamma, \gamma, B$, s, etc. are given on the basis of known experimental data.

From the equilibrium value of the TP Eq. (1), taking into account Eqs. (2) and (3), the following relations can be obtained for the magnetic part of the entropy of the AFM phase:

$$S_{AF} = \frac{1}{2} Nk(\ln Z(y) - \sigma y), \qquad (4)$$

and the entropy of the lattice (phonons) (see also [21]):

$$S_{\rm ph} = -Nk \left(3 \ln \left(1 - e^{-\frac{\Theta}{T}} \right) - 4D \right), \tag{5}$$

Eq. (2–5) were used in the present work to calculate the magnetic properties of FeRh alloy.

2.2. Calculation of the FM phase properties

In this paper we consider FeRh with two sublattices of atoms: a sublattice of Rh atoms with reduced magnetization σ_{Rh} and a sublattice of Fe atoms with reduced magnetization σ_{Fe} . This is an equiatomic ordered alloy with magnetic Fe atoms (spin $s_{Fe} = 3/2$) and Rh (spin $s_{Rh} = 1/2$).

The thermodynamic potential of the FM phase has the form:

$$F = \frac{1}{2} N_{1} J_{11}^{f} s_{Rh}^{2} \sigma_{Rh}^{2} + \frac{1}{2} N_{2} J_{22}^{f} s_{Fe}^{2} \sigma_{Fe}^{2} + N_{1} J_{12}^{f} \sigma_{Rh} \sigma_{Fe} s_{Rh} s_{Fe}$$

- $N_{1} kT (\ln Z(y_{3}) + \ln Z(y_{4})) + \frac{1}{2} B \omega^{2} + P \omega$
+ $N kT \left(3 \ln(1 - e^{-\Theta/T}) - D \left(\frac{\Theta}{T}\right) \right) - N_{1} g \mu s_{Rh} H - N_{2} g \mu s_{Fe} H,$ (6)

where $J_{11}^{f} = J_{110} + \gamma_{11}\omega$, $J_{22}^{f} = J_{220} + \gamma_{22}\omega$, $J_{12}^{f} = J_{120} + \gamma_{12}\omega$, $\Theta = \Theta_{0} - \Gamma\omega$, $y_3 = \left(\frac{s_{Fe}}{kT}\right) [g\mu H + J_{11}^f s_{Rh} \sigma_{Rh} + J_{12}^f s_{Fe} \sigma_{Fe}],$ $y_4 = \left(\frac{s_{Fe}}{kT}\right) [g\mu H + J_{22}^f s_{Fe} \sigma_{Fe} + J_{21}^f s_{Rh} \sigma_{Rh}],$

 J_{ii}^{f} are the exchange integrals between an atom of type *i* (where i = 1 means Rh, i = 2 means Fe) and all atoms of type *j* (where j = 1means Rh, j = 2 means Fe) in the FM phase. N_1 and N_2 are the number of atoms per unit volume for Rh and Fe sublattices, respectively. $N_1 =$ $N_2 = N/2$. From the condition of the minimum of the TP Eq. (6), the equilibrium equations of state for the magnetic subsystem and volume can be obtained from the magnetizations of the sublattices σ_{Rh} , σ_{Fe} and ω:

$$\sigma_{\rm Rh} = B_{\rm s_{\rm Rh}}(y_3), \, \sigma_{\rm Fe} = B_{\rm s_{\rm Fe}}(y_4) \tag{7}$$

$$\omega_{\rm F} = \frac{1}{2} (N_1 \gamma_{11} s_{\rm Rh}^2 \sigma_{\rm Rh}^2 + N_2 \gamma_{22} s_{\rm Fe}^2 \sigma_{\rm Fe}^2 + 2N_1 \gamma_{12} \sigma_{\rm Rh} \sigma_{\rm Fe} s_{\rm Rh} s_{\rm Fe}) B^{-1} + 3 \frac{N k T}{\Theta} \Gamma D \left(\frac{\Theta}{T}\right) B^{-1} - P B^{-1}$$
(8)

The appropriate formula can be obtained for the magnetic part of the entropy of the FM phase:

$$S_{\rm F} = \frac{1}{2} \mathrm{Nk} [(\ln Z(y_3) - \sigma_{\rm Rh} y_3) + (\ln Z(y_4) - \sigma_{\rm Fe} y_4)]$$
(9)

The entropy of the FM phase of FeRh alloy is also contributed by the lattice entropy described by Eq. (5). However, the numerical values of S_F from Eq. (5) will differ for FM and AFM phases, since these phases have different dependences ω (T) and Θ (T).

3. Application of the model for numerical calculation

By Eqs. (1)–(5) and Eqs. (6)–(9), numerical calculations of the following properties of FeRh alloy for the AFM and FM phases were carried out: the temperature dependence of the reduced magnetization σ (T), the temperature dependence of the relative change in volume and magnetic entropy, and the dependence of the Néel temperature on pressure.

In numerical calculations, the experimental results from the following papers [3,29–31,33] were used. From these papers, we have: a $\approx 3\cdot 10^{-8}$ cm, $N=2/a^3=7.4\cdot 10^{22}$ cm $^{-3}$, $B=2\cdot 10^{12}$ erg/cm 3 , $\Theta_0=400$ K, $\Gamma=800$ K, s=3/2. In Ref. [3] it was theoretically shown that for an ideal defect-free structure of stoichiometric, completely B2-ordered FeRh, the AFM-FM transition point is observed at 495 K. When additionally considering the effect of Fe "anti-site" defects of 2% value transition temperature decreases to 415 K. The value of 400 K was used as some conditional average value between the theoretical results of [3] and the experimental results obtained on real samples. The constant Γ is related to the dimensionless Grüneisen constant γ' by the relation $\gamma'=\Gamma/\Theta_0$. According to Ref. [34], $\gamma'\approx2$. In numerical calculations, the following values of the parameters entering into Eqs. (1)–(3) are also accepted: $J_{11}^0=2.35\times 10^{-14}$ erg, $J_{12}^0=-2.98\times 10^{-14}$ erg, $\gamma=1\times 10^{-12}$ erg.

The exchange integrals with index 0 in the AFM phase (J_{11}^{0}) and J_{12}^{0} are the exchange integrals $J_{11} \mu J_{12}$ in the AFM phase at zero value of the relative volume change ω . J_{110} , $J_{120} \mu J_{220}$ are the exchange integrals in the ferromagnetic phase J_{11}^{f} , J_{12}^{f} and J_{22}^{f} at a zero value of ω . The constant of magnetoelastic interaction determines the dependence of the exchange integral J_{12} in the AFM phase on the volume. The constants γ_{11} , γ_{12} and γ_{22} determine the dependence of the exchange integrals J_{11}^{f} , J_{12}^{f} and J_{22}^{f} , on volume, respectively.

In addition, for the FM phase we have: $J_{110} = 7 \times 10^{-14}$ erg, $J_{220} = 3 \times 10^{-14}$ erg, $J_{120} = 10.3 \times 10^{-14}$ erg, $B = 2 \times 10^{12}$ dyn/cm², $\Theta_0 = 400$ K, $\Gamma = 800$ K. Here, the elastic and thermal properties of the paramagnetic AFM and FM phases are assumed to be the same (B, Θ_0 and Γ are the same for these phases).

The parameters of the magnetoelastic interaction are chosen in such a way as to have suitable (close to experiment) values of the volume magnetostriction and the dependences of the T_C and T_N on the pressure: $\gamma_{11} = 1 \times 10^{-12}$ erg, $\gamma_{12} = 0.4 \times 10^{-12}$ erg, $\gamma_{22} = 0.1 \times 10^{-12}$ erg.

It should be noted that the choice of the numerical values of the above-mentioned exchange integrals and constants of the magnetoe-lastic interaction is ambiguous. Since there are no data from independent sources about their values, they were chosen in such a way as to obtain the Neel and Curie temperatures close to those observed in the experiment. The numerical values of the constants γ_{11} , γ_{12} , γ_{22} and γ are chosen so as to obtain close to the experimentally observed values of $\omega \sim 10^{-2}$.



Fig. 1. Temperature dependence of the reduced magnetization. 1 – reduced magnetization of AFM phase $\sigma(T)$. 2 and 3 – numerical curves of $\sigma_{Fe}(T)$ and $\sigma_{Rh}(T)$, respectively.

4. Results and discussion

Numerical calculations begin with the solution of the transcendental equation Eq. (2) and the system of equations Eq. (7). Thus, the temperature dependences of the reduced magnetization of one sublattice of Fe atoms in the AFM phase of σ (T) from Eq. (2) are determined as well as the dependences σ_{Rh} (T) and σ_{Fe} (T) from Eq. (7) for the FM phase. The Néel temperature T_N is determined from the condition σ (T_N) = 0, and T_C is determined from the equalities σ_{Rh} (T_C) = σ_{Fe} (T_C) = 0. The result of solving Eq. (2) and Eq. (7) is shown in Fig. 1. For a phase transition at the Néel point (T_N = 405 K), a first-order phase transition is obtained, which is a consequence of the strong magnetoelastic interaction in the AFM phase. For the FM phase, we get a second-order phase transition at $T_C = 670$ K (Fig. 1).

Fig. 2 shows the results of calculating the temperature dependence of one sublattice magnetization in the AFM phase $(M_1 = -M_2 = 2\mu_{S_Fe}\sigma_4^N)$ and the magnetization of the FM phase $(M = 2\mu_{S_Rh}\sigma_{Rh}\frac{N}{2} + 2\mu_{S_Fe}\sigma_{Fe}\frac{N}{2})$. The result of the calculation (curve 2 in Fig. 2) is in good agreement with the experimental data (Fig. 1 of [7]). Our calculation of magnetization is performed at zero magnetic field. Such a calculation represents the spontaneous magnetization of the sample, since in our theory it is assumed that the sample is single-domain and there is no magnetic anisotropy. Such a calculation should be



Fig. 2. Temperature dependence of magnetization. 1 – magnetization of Fe atoms sublattice in the AFM phase $(M_1 = -M_2 = 2\mu s_{Fe}\sigma N/4)$. 2 – magnetization in the FM phase $(M = 2\mu s_{Rh}\sigma_{Rh}\frac{N}{2} + 2\mu s_{Fe}\sigma_{Fe}\frac{N}{2})$.



Fig. 3. Temperature dependence of the relative volume change: AFM (1), PM (2), FM (3).

compared with the experiment, which allows one to exclude the influence of the domain structure and magnetic anisotropy. Approximately, these conditions can be obtained in larger magnetic fields. Thus, we make a comparison with M (T) for a field of 14,500 Oe, shown in Fig. 1 in Ref. [7]. A good agreement is observed both qualitatively (according to the nature of the dependence) and according to the maximum magnitude of the magnetization (after reduction to the same units).

Using the known values of σ (T), $\sigma_{\rm Rh}$ (T) and $\sigma_{\rm Fe}$ (T), it is possible to calculate the equilibrium values of different thermodynamic quantities. Fig. 3 shows the temperature dependence of the relative change in volume for the AFM, FM, and PM phases of the FeRh alloy calculated by Eq. (3) and Eq. (8). With the above numerical values of the constants of the magnetoelastic interaction, we obtained $\omega_{AF}(0 K) \approx -2 \times 10^{-2}$ and $\omega_F(0 K) \approx 1 \times 10^{-2}$. At the same time, it should be noted that in traditional antiferromagnetic materials, such as terbium, there is a sharp increase in the volume magnetostriction in the region of the FM-AFM and AFM-PM transitions [35].

In the model used, negative SVM for the AMF phase and positive SVM for the FM phase are adopted. This choice provides agreement with the experimental results of [36] for the dependence of the Néel and Curie temperatures (an increase in T_N and a decrease in T_C with increasing pressure). Fig. 4 shows the result of calculating the dependence of T_N and T_C on pressure.

The calculated values of the magnetic and total entropies of the



Fig. 4. Pressure dependences of the Néel and Curie temperatures.



Fig. 5. Temperature dependence of the magnetic entropy change for the AFM (1) and FM (2) phases.



Fig. 6. Temperature dependence of the full entropy change for the AFM (1) and FM (2) phases. The Néel temperature is marked with an arrow.

AFM and FM phases of the FeRh alloy are shown in Fig. 5 and Fig. 6. The calculation is performed using Eqs. (4) and (5) and Eq. (9). The total entropy is the sum of the magnetic and lattice contributions. The difference $S_F - S_{AF} \approx 1.2 \times 10^6$ erg/cm³ K for magnetic entropy, and the difference $S_F - S_{AF} \approx 2 \times 10^6$ erg/cm³ K for the full entropy are calculated for the temperature of 1st order magnetic phase transition T = 350 K. One should note that the general character of the magnetic part of entropy dependence on temperature is typical for anti-ferromagnetic materials e.g. in single-crystalline Dy (see Fig. 4 of [37]).

In typical rare-earth antiferromagnets, thermodynamic potentials include the free energy of the exchange interaction between the layers, the magnetoelastic and the exchange energy. The heat released in the magnetic field during the AFM-FM transition is released due to positive contributions from changes in the exchange energy, magnetoelastic energy and anisotropy energy, as well as a negative contribution due to overcoming the energy barrier during the transition. Mainly, heat release is caused by a change in exchange and magnetoelastic energy (e.g. in single-crystalline Dy (see Table 2 of [38]). Thus, it was also interesting to calculate the thermodynamic potential as a function of temperature within this model. The temperature dependence of the thermodynamic potentials of the AFM (Eq. (1)) and the FM phase (Eq. (6))



Fig. 7. Temperature dependence of the thermodynamic potentials of the AFM (1) and the FM phase (2).

(at H = 0, P = 0) is shown in Fig. 7.

The absence of an intersection of the temperature dependences of thermodynamic potentials (Fig. 7) is due to the fact that the model does not take into account the influence of the sublattice of Rh atoms in the AFM phase. This in turn indicates that within the framework of this model, the cause of the AFM - FM phase transition in FeRh is the appearance of a nonzero magnetic moment on Rh atoms with an increase in the lattice volume in combination with a decrease in the absolute value of the exchange integral J_{12} .

The presented model satisfactorily describes some of the magnetic and thermal properties of the FeRh alloy. The AFM - FM transition point in FeRh alloys is extremely sensitive to the alloy composition and the presence of defects in the alloy [3,4]. For example, ab initio calculations [3] show the transition temperature value close to 495 K for stoichiometric completely B2-ordered FeRh alloy with an ideal structure without any defects. "Anti-site" defects' addings to the model used in Ref. [3] leads to the decrease of transition temperature in FeRh. Thus, the transition temperatures in real alloys turn out to be lower than theoretical calculations show for ideal compositions. Experimental results show that the phase transition temperature in FeRh alloys ranges from RT to 400 K. Such a large difference in transition points is due to the strong dependence of T_N on many factors, such as alloy composition, alloy preparation procedures, heat treatment, and the presence of defects etc. In case of FeRh films, the transition temperature also depends on the film thickness and the presence of lattice strain [39,40]. When applying our model to FeRh alloys at the end of the article, we used a transition temperature of 350 K as the average of the range of transition temperatures obtained experimentally on real alloys. The estimates made are in good agreement with the experimental results obtained for real FeRh alloys. The 1st order magnetic phase transition (AFM-FM transition) occurs at $\sim T = 350$ K. Then, according to our estimates, at the transition point: $\Delta S = S_F - S_{AF} \approx 2 \times 10^6 \text{ erg/cm}^3 \text{K}$, $\Delta M \approx 130 \text{ emu/g} = 1300 \text{G}, \Delta V/V \approx 1.7 \times 10^{-2}$

With these values from the Clausius-Clapeyron relations:

$$\frac{\partial T_{AF}}{\partial P} = \frac{\Delta V}{V} \frac{1}{\Delta S} = \frac{\Delta \omega}{\Delta S}, \quad \frac{\partial H_C}{\partial T} = -\frac{\Delta S}{\Delta M}, \quad (10)$$

where, H_C is the critical magnetic field causing the AFM-FM transition, one can obtain $\frac{\partial T_{AF}}{\partial P} \approx 8 \times 10^{-3}$ K/atm, $\frac{\partial H_C}{\partial T} \approx -1.5 \times 10^3$ Oe/K, which is in good agreement with the experimental results [29].

5. Conclusions

The application of the exchange-striction model for calculation of

the magnetic properties (temperature dependence of the relative volume change, the dependence of T_N and T_C on pressure) of the AFM and FM phases in Fe–Rh alloy is proposed. It is demonstrated that the assumption of negative spontaneous volume magnetostriction in the AFM state and positive spontaneous volume magnetostriction in the FM phase leads to a good agreement between the theory and the experimental data. The model is planned to be expanded taking into account the contribution of the collectivized electrons of Rh and Fe atoms in the AFM phase.

Acknowledgements

This work was supported in part IMP Neutron Material Complex within state assignment of FASO of Russia (theme "Flux" no. AAAA-A18-118020190112-8). Work in Advanced Magnetic TechnolC is supported bogies and Consulting, LLy Skolkovo Foundation, Russia.

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