

*Physics*

## Temperature Dependence of Hydrogen Mobility in Ordering Rare-Earth Dihydrides

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**ABSTRACT.** The rare-earth ordering dihydrides are considered. The influence of ordering processes on the mobility of interstitial H-atoms is investigated. It is shown that those H-H interactions which induce formation of ordered superstructures in the hydrogen sublattice, provide as well the increment of the dwell time of the moving particles. The latter effect can be interpreted as a “weighting” of mobile H-atoms. The influence of the “particle-weighting effect” on the temperature dependence of the dipole-dipole interaction induced nuclear spin-lattice relaxation time is examined. It is shown that although the corresponding changes in the  $T_{ld}(T)$  curve are remarkable, their influence on the total  $T_l(T)$  dependence, determined as well by interactions of nuclear spins with conduction electrons, is negligibly small. © 2009 Bull. Georg. Natl. Acad. Sci.

**Key words:** metal hydrides, ordering processes, hydrogen “weighting”; nuclear spin-lattice relaxation.

**The model and general relations.** It is well known that in a number of M-H compounds (metal-hydrogen interstitial alloys) the temperature lowering provides formation of ordered superstructures in the subsystem of hydrogen atoms (H-atoms). Inelastic neutron scattering experiments had established that in such ordering hydrides the frequencies of local vibrations of interstitial H-atoms significantly decrease below the disorder-order transition temperature [1]. The local vibration frequencies  $\nu(\text{loc})$  are directly related to the time-parameter  $\tau_0$  describing the hydrogen “from site – to site” jumping processes. The same time-parameter  $\tau_0$  turns out to be an essential part of expressions describing the spin-lattice relaxation processes caused by the dipole-dipole interactions of the spins of hydrogen and metal nuclei [2, 3]. In the latter case  $\tau_0$  is usually assumed to be constant in the whole temperature range under consideration. There arises therefore a natural question - what type of modifications can be expected in the temperature dependence of the spin-lattice relaxation time

$T_l(T)$  if we take into account the temperature variations of  $\tau_0$  parameter. We intend to discuss this problem in the given investigation consisting of two parts. In the first one we consider the interrelations between the hydrogen ordering processes and the temperature dependence of the time parameter  $\tau_0$ , while in the second part we shall estimate the degree of changes in the spin-lattice relaxation rates caused by the obtained  $\tau_0(T)$  dependence.

As an example we consider the ordered rare-earth dihydrides  $\text{MH}_{2+c}$  ( $0 < c < c_{\text{max}}$ ;  $c_{\text{max}} \leq 1$ ), where  $N$  metal atoms form a *fcc* lattice,  $2N$  hydrogen atoms fill the set of  $2N$  tetrahedral interstitial positions ( $\text{H}_T$ -atoms), while the remaining  $cN$  H-atoms ( $\text{H}_O$ -atoms) are distributed among  $N$  octahedral interstitial positions. Just the latter part of hydrogen atoms reveal a considerably high mobility (with respect to  $\text{H}_T$ -atoms) and form the ordered superstructures at temperatures lower than the disorder-order transition point  $T_{lr}$ . The ordered superstructures formed, particularly, in lanthanum dihydrides are described by two long-range-order pa-

rameters ( $\eta_1$  and  $\eta_2$ ), and reveal a step-wise ordering process involving disorder-order and order-order transition points,  $T_{tr1}$  and  $T_{tr2}$ . In case of the compound under consideration,  $\text{LaH}_{2.27}$ ,  $T_{tr1} = 365$  K and  $T_{tr2} = 343$  K, respectively (see e.g. [4]). The development of the ordering process subdivides the total set of octahedral positions into three groups of sites, which differ by the occupation probabilities, or, in other words, by the “sites occupation numbers” -  $n_1$ ,  $n_2$  and  $n_3$ , related to the order parameters  $\eta_1$  and  $\eta_2$  [5]:

$$n_1 = c + \eta_1 g + 2\eta_2 g, n_2 = c + \eta_1 g - 2\eta_2 g, n_3 = c - \eta_1 g. \quad (1)$$

where  $g = 0.25$  is a normalizing factor which provides the occupation numbers to be located within the physically meaningful range  $[0 \leq n_1, n_2, n_3 \leq 1]$ . The differences between occupation numbers arise at temperatures below the transition points  $T_{tr1}$  and  $T_{tr2}$  (see Fig. 1).

The internal energy of the ordering subsystem can be written in the following form [5]

$$E(c, T) = [N k_B / 2] [V(0)c^2 + V(\mathbf{k}_1)(\eta_1(T)g)^2 + 2V(\mathbf{k}_2)(\eta_2(T)g)^2], \quad (2)$$

Here  $\mathbf{k}_1$  and  $\mathbf{k}_2$  are the wave vectors of the distribution function describing the equilibrium superstructure, while  $V(0)$ ,  $V(\mathbf{k}_1)$  and  $V(\mathbf{k}_2)$  are the H-H interaction potential Fourier-components (taken in temperature units). Numerical values of the energy parameters  $V(0)$ ,  $V(\mathbf{k}_1)$  and  $V(\mathbf{k}_2)$  are defined basing on experimental data. Particularly, it was established [4, 6] that for the superstoichiometric dihydrides of lanthanum the energy parameter  $V(\mathbf{k}_1)$  can be estimated from the relation  $T_{tr1} = -V(\mathbf{k}_1)c(1-c)$ , which for  $c = 0.27$  and  $T_{tr1}(\text{LaH}_{2.27}) = 365$  K, gives us  $V(\mathbf{k}_1) = -1853$  K [4], while for the ratio of energy constants  $[V(\mathbf{k}_2)/V(\mathbf{k}_1)] \equiv p$  the value was determined:  $p = 0.7743$  [6]. The energy parameter  $V(0)$  remains unknown, but as we are interested in the temperature variations of the ordering system with a fixed concentration, the latter parameter is less important and we shall assume that  $V(0) = 0$ .

Some words about the energy ascribed to the local vibrations of  $\text{H}_0$ -atoms. It was defined as  $E_0(\text{loc}) = \hbar\nu(\text{loc})$  and determined from the diffuse inelastic neutron scattering data [7, 8]. For our numerical estimations a tentative value  $E_0(\text{loc}) \approx 100$  meV was selected, or in the temperature units,  $E_0(\text{loc}) = 1160$  K.

The dipole-dipole interaction of the mobile proton spins with the nuclear spins of surrounding metal atoms and those of the remaining  $\text{H}_0$  and  $\text{H}_T$  atoms induces the spin lattice relaxation process characterized by the temperature-dependent relaxation time  $T_{1d}$ . The latter is usually described by an expression [2, 3] which can be

schematically presented in the following form

$$T_{1d}^{-1} = \tau [J^H(T)\Sigma_j^H + J^M(T)\Sigma_j^M], \quad (3)$$

where  $J^H(T)$  and  $J^M(T)$  are the temperature-and-time-dependent factors, while  $\Sigma_j^H$  and  $\Sigma_j^M$  denote the sums of functions of the distances separating the resonating H-particle from the surrounding hydrogen and metal atoms, respectively, while  $\tau$  denotes the dwell time of jumping  $\text{H}_0$ -atoms (i.e.  $\tau^{-1}$  is the number of the site-to-site jumps in a time unit).

The redistribution of H-atoms in the metal lattice occurs at temperatures well above the low-temperature range, where the quantum diffusion dominates. For this reason we describe the hydrogen motion within the metal lattice as an activation process characterised by an activation energy  $E_a$ . In these conditions the dwell-time  $\tau$  of the moving particle can be presented as

$$\tau = \tau_0 \exp(E_a/k_B T), \quad (4)$$

where  $\tau_0$  is usually supposed to be constant in the whole temperature range under consideration.

The dwell-time  $\tau$  was defined above as inversely proportional to the particle's jumping frequency  $\nu$ . A potential barrier overcome implies that  $\nu = \nu_0 \exp[-E_a/k_B T]$ , where  $\nu_0$  is the jumping frequency at extremely high temperatures and is proportional, on the one hand, to the local oscillation frequency  $\nu(\text{loc})$ , and, on the other - to  $\nu_0 = (\tau_0)^{-1}$ . Thus we have

$$\tau_0 \sim \nu(\text{loc})^{-1}. \quad (5)$$

Let us consider the behavior of an H-atom local frequency  $\nu(\text{loc})$  during the ordering process. For clarity, we shall consider a simplest example of a quantum one-dimensional oscillator which moves in the field given by the potential function  $V(x) = Kx^2/2$ . The quantum state of such a particle is described by the Schrödinger equation:

$$[\partial^2/\partial x^2]\psi(x) + [(2m\epsilon/\hbar^2) - (mKx^2/\hbar^2)]\psi(x) = 0. \quad (6)$$

The eigenvalues of this equation are well known:

$$\epsilon \equiv \epsilon_0 = \hbar\omega_0(n + 1/2), \quad \text{where } \omega_0 \equiv \sqrt{(K/m)}, \quad (7)$$

and  $n$  are integers. In this case  $\nu(\text{loc}) \equiv \nu(\text{loc})_0 = (1/2\pi)\sqrt{(K/m)}$ .

Those H-H interactions, which cause spatial redistribution of H-atoms in the ordering metal hydrides, can be considered to be responsible for the H-atom's local frequency changes. **In order to account for this perturbation phenomenon let us introduce in (6) a corresponding potential  $V_{HH}$  and assume that  $V_{HH}$  is proportional to the  $(1/cN)$  part of the ordering energy of  $\text{H}_0$ -atoms  $E(c, T)$ ,**

$$V_{HH} \sim (1/cN)E(c, T), \quad (8)$$

then (6) will take the form

$$[d^2/dx^2]\psi(x) + [(2m(\varepsilon - V_{HH})/\hbar^2) - (mKx^2/\hbar^2)]\psi(x) = 0. \quad (6')$$

Taking into account that the additional term  $V_{HH}$  can be as large as the oscillator energy  $\varepsilon_0$ , the traditional perturbation theory cannot be used, and we shall try to account for this perturbation by a corresponding renormalization of the mass of oscillating particles. The following obvious mathematical transformations give:

$$m(\varepsilon - V_{HH}) = m\varepsilon(1 - V_{HH}/\varepsilon) \equiv m^*\varepsilon; \quad m^* \equiv m(1 - V_{HH}/\varepsilon). \quad (9a)$$

$$mK \equiv K[m^*/(1 - V_{HH}/\varepsilon)] = K^*m^*, \quad K^* = K(1 - V_{HH}/\varepsilon)^{-1}. \quad (9b)$$

Using these new notations, equation (3') will take a shape coinciding formally with (3), and its eigenvalues will coincide outwardly with those given by (4). We shall have

$$[d^2/dx^2]\psi(x) + [(2m^*\varepsilon/\hbar^2) - (m^*K^*x^2/\hbar^2)]\psi(x) = 0. \quad (10)$$

$$\varepsilon = \hbar \omega_H(T)(n + 1/2), \quad (11)$$

where

$$\omega_H(T) = \omega_0(1 - V_{HH}/\hbar\omega_0)^{-1}. \quad (12)$$

Within the high-temperature disordered state the ordering energy of  $H_O$ -atoms  $E(c, T)$  is zero and the local mode frequency has to be presented by its traditional expression -  $\nu(\text{loc})_0 = (1/2\pi)\sqrt{(K/m)}$ . When temperature is lowered below the disorder-order transition point, then  $E(c, T)$  becomes negative and following relations (8) and (12) it has to be concluded that  $\nu(\text{loc})$  will become lower than  $\nu(\text{loc})_0$ . Thus, it follows that formation of an ordered state provides temperature variations of the time parameter  $\tau_0$  - it increases monotonically at temperature lowering.

A detailed numerical analysis of the corresponding changes in the spin-lattice relaxation time performed for the ordering lanthanum dihydride  $\text{LaH}_{2.27}$  will be given below. Here we present only intermediate numerical results characterizing the H-H interaction induced temperature variations of the  $\tau_0$ -factor in the selected M-H compound. Particularly, we present in Fig. 1 the ordered state formation process (by giving the temperature changes of occupation numbers  $n_1, n_2$  and  $n_3$ ), in Fig. 2 - temperature dependence of the ordering energy  $E(c, T)$ , and in Fig. 3 - the calculated  $\tau_0(T)$  dependence.

As a concluding remark we can formulate the following statement.

Formation of ordered superstructures in ordering metal-hydrogen systems is accompanied by the H-H

interaction induced hydrogen mobility reduction, which can be interpreted as some "effective weighting" of spatially ordered particles.

**Application to spin-lattice relaxation processes in the rare-earth metal dihydrides.** Numerical estimations of the spin-lattice relaxation time  $T_1(T)$  are performed for the lanthanum dihydride  $\text{LaH}_{2.27}$ , where the subsystem of hydrogen atoms located in the octahedral interstitial positions (the subsystem of  $H_O$ -atoms) undergoes a two-step disorder-order type phase transformation and forms a sequence of ordered spatial configurations. For simplicity we assume that spatial redistribution of  $H_O$ -atoms do not influence neither on the metal *fcc* lattice, nor on the equilibrium states of the remaining part of H-atoms located in the tetrahedral interstitial positions ( $H_T$ -atoms).

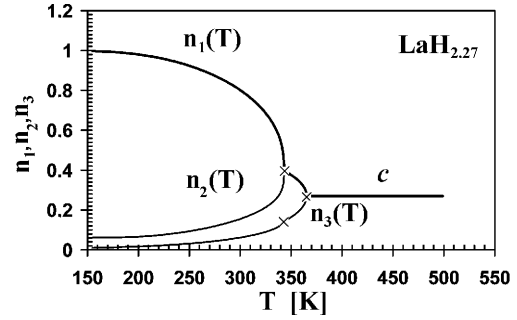


Fig. 1. Formation of an ordered configuration in the subsystem of  $H_O$ -atoms;  $n_1(T)$ ,  $n_2(T)$  and  $n_3(T)$  are the sites occupation numbers (the sites occupation probabilities).

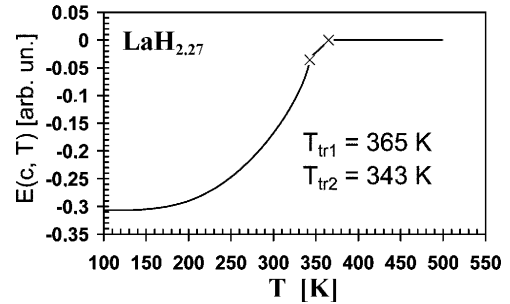


Fig. 2. The internal ordering energy  $E(c, T)$  of the system of  $H_O$ -atoms.

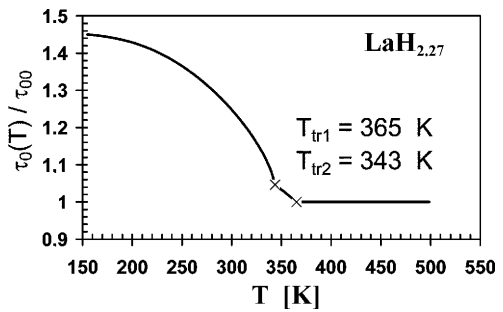


Fig. 3. H-H interaction induced temperature variations of  $\tau_0$  time-parameter ( $\tau_{00}$  denotes the unperturbed, high-temperature value).

In a pure (undoped) nonmagnetic metal hydride the experimentally determined spin-lattice relaxation rate  $R_1 \equiv (1/T_1)$  is a summary of two relaxation processes – the first one, based on the dipole-dipole interactions of hydrogen and metal nuclear spins, is characterized by the dipolar relaxation time  $T_{1d}$ , and the second one, based on the contact interaction of the proton and electron spins (the so-called “Korringa-interaction”), is characterized by the relaxation time  $T_{1e}$ . Mathematical relations which describe the corresponding relaxation processes are well known and they were intensively applied to the analyses of experimentally investigated different metal hydrides (see e.g. [2-4, 9-11]). Particularly, the relaxation time  $T_{1e}$  caused by the contact interaction of the mobile  $H_O$ -atoms with conduction electrons, is described usually by the Korringa relation

$$T_{1e}(T) = K_{\text{kor}}/T, \quad K_{\text{kor}} = \text{const}, \quad (13)$$

while the dipole-dipole interactions of the mobile proton spins with the nuclear spins of surrounding metal atoms and those of the remaining  $H_O$  and  $H_T$  atoms, are described by the set of following expressions [2-4, 9-11]:

$$\begin{aligned} [1/T_{1d}] = & (2/5)(C_I/\omega_I) y \{ [(1/[1+y^2]) + (4/[1+(2y)^2])] \times \\ & \times [\Sigma_i^{HT}(1/r_i^H)^6 + \Sigma_i^{HO} n(i) (1/r_i^H)^6] + (C_S/C_I) [(1/3) \times \\ & \times (1/[1+k_1 y^2]) + (1/[1+y^2]) + (2/[1+k_2 y^2])] \Sigma_i^m (1/r_i^m)^6 \}, \end{aligned} \quad (14)$$

where

$$y \equiv \omega_I \tau, \quad \tau = \tau_0 \exp[E_a / k_B T], \quad (15a)$$

$$k_1 \equiv (1 - (\omega_S/\omega_I))^2, \quad k_2 \equiv (1 + (\omega_S/\omega_I))^2; \quad (15b)$$

$$\begin{aligned} C_I = & \gamma_I^4 \hbar^2 I(I+1), \quad C_S = \gamma_S^2 \gamma_S^2 \hbar^2 S(S+1); \\ \omega_I = & \gamma_I H_0, \quad \omega_S = \gamma_S H_0; \end{aligned} \quad (15c)$$

In the relation (14) symbols  $\Sigma^m$ ,  $\Sigma^{HT}$  and  $\Sigma^{HO}$  denote, respectively, the sums over the metal lattice sites, and the two types of interstitial positions occupied by H-atoms. It is assumed that the sums  $\Sigma_i^m (1/r_i^m)^6$  and  $\Sigma_i^{HT} (1/r_i^H)^6$  are constant over the whole temperature range, while the sum  $\Sigma_i^{HO} n_i (1/r_i^H)^6$  contains the temperature-dependent factors  $n_i \equiv n_i(T)$  denoting the occupation numbers of interstitial positions, which change significantly in the vicinity of the disorder-order transition points. (An example of the temperature dependence of occupation numbers in the ordering system is shown in Fig. 1). In expressions (15) numerical parameters  $(\gamma_I, \omega_I)$  and  $(\gamma_S, \omega_S)$  represent, respectively, the gyromagnetic ratios and Larmor frequencies of interstitial H-nuclei (with spin  $I$ ) and those of metal M-nuclei (with spin  $S$ ). In expressions (15a)  $\tau$  is the dwell-time of the

jumping H-atoms. (If the mobility of H-atoms is characterized by the number of site-to-site jumps  $\nu$ , then  $\tau = \nu^{-1}$ .  $E_a$  is the corresponding activation energy, and  $\tau_0$  is the “preexponential factor”).

In summarizing the mathematical scheme of calculations we formulate:

$$R_1 = R_{1d} + R_{1e}, \quad (16)$$

where  $R_{1e} \equiv (1/T_{1e})$  is determined by the relations (13), and  $R_{1d} \equiv (1/T_{1d})$  is given by the expressions (14)-(15).

Following equation (14), the development of an ordering process in M-H compounds should be reflected, first of all, in the temperature dependence of the sum  $\Sigma_i^{HT} \Sigma_i^{HO} n_i(T) (1/r_i^H)^6$ . In [4] we had analyzed the experimental data [10] obtained on the ordering lanthanum dihydride  $\text{LaH}_{2.27}$ , and had established that the given mathematical refinement of the corresponding calculations provides a negligibly small influence on the numerical values of the summary dependence  $T_1(T)$ .

Now we examine the influence of the above established  $\tau_0(T)$  dependence on the dipole-dipole interaction induced part of the spin-lattice relaxation time  $T_{1d}(T)$  and on the total relaxation time  $T_1(T)$ . Estimations of tentative temperature changes of the  $\tau_0$  parameter values were shown in the corresponding figure (see Fig. 3) and they turned out to be sufficiently significant, but there remains a question – in what degree the calculated values of the spin-lattice relaxation time are influenced by taking into account the temperature variations of  $\tau_0$  parameter

It is obvious that the increment of the time spent by each of the moving particles at the visited sites (the increment of the dwell-time) will cause an increment of the corresponding  $T_{1d}(T)$  values. This natural conclusion is justified by the results of numerical estimations presented in Fig. 4. The next question is – how can the resulting changes in the general temperature dependence of the dipole-dipole relaxation time  $T_{1d}(T)$  be classified. From Fig. 5 it follows that these changes are *remarkable, but not essential*. Very significant is the fact that they are revealed in the low temperature range, where the total rate of the nuclear spin relaxation process is determined mainly by interactions of nuclear spins with conduction electrons. The latter statement is illustrated in Fig. 6. Here both calculated dependences  $T_{1e}(T)$  and  $T_{1d}(T)$  are denoted by corresponding thin lines, while the thick line presents the calculated resulting  $T_1(T)$  dependence.

From the above short consideration two qualitative conclusions may be deduced.

- 1) In the case of ordering lanthanum dihydrides,

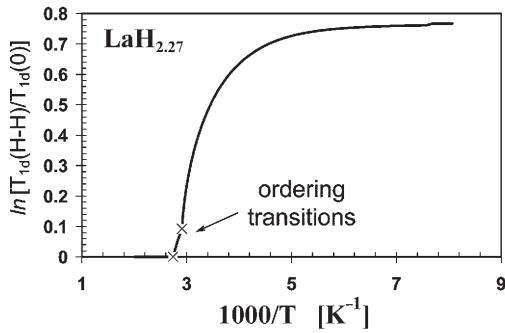


Fig. 4. Temperature dependence of the difference between  $T_{1d}(T)$  values calculated in different conditions: on assuming a constant  $\tau_0$ -factor,  $T_{1d}(0)$ , and on taking into account H-H interaction induced  $\tau_0(T)$  variations,  $T_{1d}(H-H)$ .

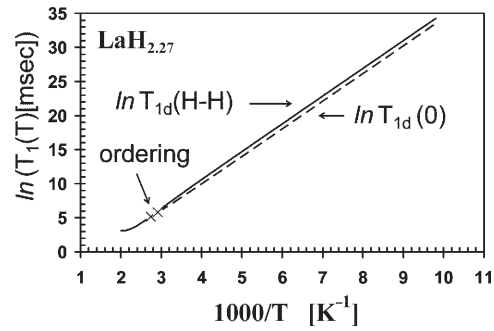


Fig. 5. Absolute values of dipole-dipole relaxation times  $T_{1d}(T)$  calculated in different conditions: on taking into account the additional H-H interactions,  $T_{1d}(H-H)$ , and without the latter refinement  $T_{1d}(0)$ .

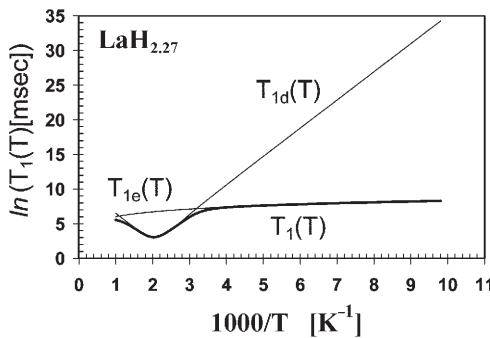


Fig. 6. Temperature dependences of the Korringa relation  $T_{1e}(T)$ , of dipole-dipole relaxation  $T_{1d}(T)$ , and of the summary relaxation time  $T_1(T)$ .

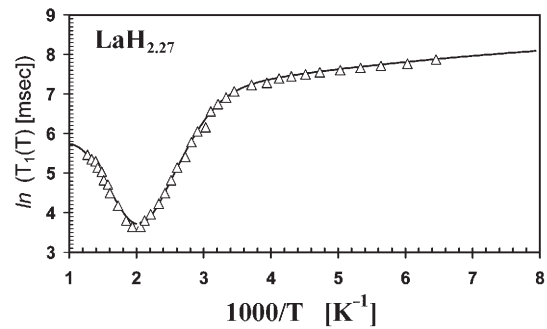


Fig. 7. Description of the sequence of experimental points by the calculated  $T_1(T)$  curve.

even in conditions of taking into account the ordering process and the “particle weighting” effect related to it, the calculated general  $T_1(T)$  dependence remains practically unchanged. It follows that the set of previously selected adjusting parameters, such as activation energy  $E_a$ , time-parameter  $\tau_0$  and Korringa constant  $K_{\text{Korr}}$ , may be left unchanged. Particularly, for the compound  $\text{LaH}_{2.27}$  successful results in the description of experimental  $T_1(T)$  dependence can be obtained on using the previously determined values of mentioned parameters [10]:

$$K_{\text{Korr}} = 410 \text{ sec K}, \quad E_a = 0.35 \text{ eV/atom},$$

$$\tau_0^{-1} = 7.4 \times 10^{11} \text{ sec}^{-1}. \quad (17)$$

In Fig. 7, we have presented experimental results [10] (the sequence of triangles) and the corresponding theoretical curve calculated basing on the given values of mentioned parameters and on taking into account simultaneously the ordering and “weighting” effects. (The calculated curve practically repeats the previously obtained theoretical dependences published in [4] and [10]).

2) It was suggested (see e.g. [11]) that in the Ce-H system, as well as in La-H system, continuous increment of the hydrogen concentration provides a smooth depleting of the conduction band. It follows that the “hydrogen nuclear spin – conduction electron spin” interaction strength will be continuously reduced as well. The band-depleting process is terminated in  $\text{LaH}_3$  and  $\text{CeH}_3$  compounds, where conduction bands turned out to be practically empty and compounds reveal the insulator (or semiconductor) properties [10]. At some lower concentration values both compounds are non-metallic in the high-temperature disordered states and reveal the ordinary metal properties in the ordered low-temperature states (below the disorder-order transition temperature). It seems natural to expect that the ordering related properties of  $\text{H}_0$ -atoms, and, particularly, the “particle weighting” effects, can be registered in the maximally proper, “unmasked” situation just in the corresponding concentration range.

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ფიზიკა

## წყალბადის ძვრადობის ტემპერატურული დამოკიდებულება იშვიათ მიწათა მოწესრიგებად წყალბადნაერთებში

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შესწავლილია მოწესრიგების პროცესის გავლენა ლითონის მესერში ჩანერგილი წყალბადის ატომების ძვრადობაზე იშვიათ მიწათა მოწესრიგებად წყალბადნაერთებში. ნაჩვენებია, რომ წყალბად-წყალბად ურთიერთქმედება, რომელიც უზრუნველყოფს მოწესრიგებული ზესტრუქტურის ჩამოყალიბებას წყალბადის ქვემესერში, ამავე დროს განაპირობებს წყალბადის ატომების კვანძთაშორის პოზიციებში დაყოვნების დროის გაზრდას, რაც შეიძლება აღიწეროს როგორც მოძრაობის ნაწილაკის “დამძიმება”. რიცხვითი შეფასებები შესრულებულია ლანთანის დიჰიდრიდისათვის  $\text{LaH}_{2.27}$  და მიღებულია აქტივაციური პროცესის დროითი პარამეტრის ტემპერატურული დამოკიდებულება. განხილულია “ნაწილაკთა დამძიმების ეფექტის” გავლენა დიპოლ-დიპოლური ურთიერთქმედებით განპირობებული ბირთვული სპინ-მესერული რელაქსაციის დროის ტემპერატურულ დამოკიდებულებაზე. ნაჩვენებია, რომ თუმცა შესაბამისი ცვლილებები  $T_{1d}(T)$  მრუდზე საკმაოდ მკვეთრია, მაგრამ ჯამურ  $T_1(T)$  დამოკიდებულებაზე, რომელიც ასევე შეიცავს ბირთვული სპინების გამტარებლობის ელექტრონებთან ურთიერთქმედების წვევსაც, ისინი პრაქტიკულად არ აისახება. ამიტომ შესაძლებელია უცვლელად იქნას დატოვებული წინათ განსაზღვრული იმ რიცხვითი პარამეტრების ერთობლიობა, რომელნიც უზრუნველყოფდნენ ექსპერიმენტული და თეორიული მონაცემების კარგ თანხვედრას.

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