

Ab initio exchange interactions and magnetic properties of $\text{Gd}_2\text{Fe}_{17}$
iron sublattice: rhombohedral vs. hexagonal phases

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Abstract

In the framework of the LSDA+ U method electronic structure and magnetic properties of the intermetallic compound $\text{Gd}_2\text{Fe}_{17}$ for both rhombohedral and hexagonal phases have been calculated. On top of that, *ab initio* exchange interaction parameters within the Fe sublattice for all present nearest and next nearest Fe ions have been obtained. It was found that for the first coordination sphere exchange interaction is ferromagnetic. For the second coordination sphere exchange interaction is observed to be weaker and of antiferromagnetic type. Employing the theoretical values of exchange parameters Curie temperatures T_C for the first as well as for the first and second coordination spheres of both hexagonal and rhombohedral phases of $\text{Gd}_2\text{Fe}_{17}$ within Weiss mean-field theory were estimated. Obtained values of T_C and its increase going from the hexagonal to rhombohedral crystal structure of $\text{Gd}_2\text{Fe}_{17}$ agree well with experiment. Also for both structures LSDA+ U computed values of total magnetic moment agree well with experimental ones.

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I. INTRODUCTION

Intermetallic compounds $R_2\text{Fe}_{17}$ with high concentration of iron (R is a rare-earth ion) are of interest for both experimental and theoretical investigations.¹ These compounds are distinct for a relatively large magnetic moment – mainly caused by the magnetic moments at the Fe ions – and comparatively low Curie temperature T_C . The compounds are crystallized in two related crystal structures – rhombohedral Th_2Zn_{17} -type and hexagonal Th_2Ni_{17} -type. In each of these structures, the Fe ions can be located in four inequivalent crystallographic positions, and for this reason various experiments reveal four values of the local magnetic moments at different positions of the Fe ions. Also, most of the intermetallic compounds $R_2\text{Fe}_{17}$ have collinear magnetic structure except for $\text{Ce}_2\text{Fe}_{17}$, $\text{Tm}_2\text{Fe}_{17}$, and $\text{Lu}_2\text{Fe}_{17}$,² where the magnetic moments of the Fe ions in all crystallographic positions are collinear to each other, but frequently antiparallel to the magnetic moments of the rare-earth ions R .

Initially, the moderate Curie temperatures T_C in the compounds $R_2\text{Fe}_{17}$ was explained on the base of assumption³ of a critical distance $r_c \approx 2.5 \text{ \AA}$ between two ions in a Fe-Fe pair, so that for the distances $r < r_c$ the exchange interaction is antiferromagnetic, whereas for $r > r_c$ – ferromagnetic. From this assumption it followed that a low value of T_C is caused by a competition of ferromagnetic and antiferromagnetic exchange interactions between neighboring pairs of the Fe ions in various crystallographic positions. It also meant that an expansion of the lattice should result in an increased number of ferromagnetic interactions and corresponding growth of T_C . Such an expansion of the lattice can be reached either inserting nonmagnetic interstitial atoms,^{4,5} or substituting the Fe ions by nonmagnetic atoms with the larger ionic radii.^{6,7}

However, in a number of experiments, for example, for substitutional solid solutions $R_2\text{Fe}_{17-x}\text{Si}_x$, it was found that the crystal lattice contracts, and T_C grows.^{8,9,10} These results question the adequacy of the simple model of exchange interactions of neighboring exchange-bounded ions that change the sign at the critical distance r_c between the ions.

To determine a relation between T_C and exchange interactions in the $R_2\text{Fe}_{17}$ series, the compound $\text{Gd}_2\text{Fe}_{17}$ is of especial interest. First, among the series $\text{Gd}_2\text{Fe}_{17}$ has the highest Curie temperature T_C . Secondly, Gd itself is located at the middle of the rare-earth series, and $\text{Gd}_2\text{Fe}_{17}$ separates the compounds with light rare-earth elements crystallizing in the rhombohedral Th_2Zn_{17} -type structure, from the compounds with heavy rare-earth ele-

ments crystallizing in the hexagonal Th_2Ni_{17} -type structure. Thus Gd_2Fe_{17} is an intriguing example among the R_2Fe_{17} series which can be found in both crystal structures.

Apparently, in most experiments samples are mixture of two structures. At the same time, there are experimental works for either pure rhombohedral structure,¹¹ or pure hexagonal structure¹² of Gd_2Fe_{17} . For Gd_2Fe_{17} in the rhombohedral structure, the values of critical temperature and saturation magnetization were found to be $T_C^{rh}=475$ K,¹¹ $M_S^{rh}=21.5 \mu_B/f.u.$,¹¹ respectively. For the hexagonal structure, these values are $T_C^{hex}=466$ K and $M_S^{hex}=21.2 \mu_B/f.u.$ ¹² Although these two sets of experimental data differ slightly and further experimental study is needed, one can notice that Gd_2Fe_{17} in the rhombohedral phase has the higher values of magnetic characteristics, than in the hexagonal one.

Motivated by this fact, in the paper we consider how the transfer from the rhombohedral to hexagonal structures in Gd_2Fe_{17} influences the values of the local magnetic moments and exchange interaction parameters. The later values are obtained using the results of electronic structure calculations within LSDA+ U method. Further values of Curie temperature were estimated in the framework of the Weiss mean-field theory. Moreover based on these calculations we propose explanation of rather low T_C values and relatively small saturation magnetization of R_2Fe_{17} series with respect to elemental bcc Fe.

II. CRYSTAL STRUCTURES AND LOCAL MAGNETIC MOMENTS

The intermetallic compound Gd_2Fe_{17} can crystallize both in the rhombohedral Th_2Zn_{17} -type structure (space group $R\bar{3}m$ – no. 166 in International Tables for Crystallography) and the hexagonal Th_2Ni_{17} -type crystal structure (space group $P6_3/mmc$ – no. 194). Main structural blocks are iron hexagons building layers. Most of these hexagons have empty centers, whereas others contain the rare-earth Gd ions or mediate the Fe ions in dumbbell positions.

The rhombohedral structure of the Th_2Zn_{17} -type is shown in Fig. 1. In this type of structure the Fe(18*f*) hexagons (let us denote Fe(18*f*) as Fe3 for the rhombohedral structure) contain the Gd ions in positions 6*c* either at the center of each hexagon, as it is presented in the upper and lower layers in Fig. 1, or alternate with empty hexagons, as it is shown in the inner two layers. Interlayer Fe(6*c*)=Fe1 ions at the dumbbell positions lower the symmetry of some iron ions in the nearest intermediate layers from 18*h* to 9*d* (above and below the

dumbbell), and hence, these intermediate layers without Gd contain ions Fe(9d)=Fe2, as well as Fe(18h)=Fe4 in the hexagons. Unit cell of the rhombohedral structure consists of one formula unit of Gd₂Fe₁₇.

The hexagonal structure of the *Th₂Ni₁₇*-type is shown in Fig. 2. In contrast with the rhombohedral structure, there are no layers where each hexagon contains the Gd ion. In this structure the Gd ions are located only at the centers of the hexagons (let us denote Fe(12j)=Fe3 for the hexagonal structure) alternating with the hexagons with the dumbbells of Fe(4f) (Fe(4f)=Fe1), and the layers with the hexagons containing Gd at each center are absent. Moreover, here one can find the alternating intermediate layers Fe(6g)=Fe2 and Fe(12k)=Fe4 without the Gd ions. Unit cell of this structure consists of two formula units of Gd₂Fe₁₇ due to the different symmetry of the rare-earth ions coordination environment in the *ab*-plane translations.

For both structures in the layers with alternating Gd-containing and empty hexagons Fe3, these hexagons are deformed – the hexagons with Gd are slightly expanded, the hexagons without Gd – contracted. Furthermore, because for the hexagons Fe2 and Fe4 the intermediate layers the Gd ion and the dumbbell Fe1 ions are alternating from one layer to another, so the ions Fe2 and Fe4 in these layers are slightly distorted upward and downward with respect to the plane, i.e. these layers are slightly corrugated.

The electronic structure of the rhombohedral structure of Gd₂Fe₁₇ was calculated in the LSDA+*U* method (Ref. 13) in the framework of the band calculation package TB-LMTO-ASA (tight-binding, linear muffin-tin orbitals, atomic sphere approximation).¹⁴ However let us mention here that only Gd 4f-shell was treated within the LSDA+*U* method since correlation effects are much stronger there than for the Fe 3d-shell ($U_{Gd} \sim 7$ eV (see below), $U_{Fe} \sim 2$ eV^{18,19}). We believe that greater part (not all) of electronic interaction effects is taken into consideration for Fe 3d-shell in the frame of LSDA approximation. It is well enough justified since responsible Stoner parameter for Fe 3d-shell $J_{Fe}^S \sim 1$ eV is close to U_{Fe} . For the hexagonal structure, the results of such a calculation were reported in Ref. 12, below we include some details of that calculation to provide the full picture for comparison of the rhombohedral and hexagonal structures of Gd₂Fe₁₇. Lattice parameters for the rhombohedral structure are $a=8.538$ Å and $c=12.431$ Å (Ref. 16), for the hexagonal structure – $a=8.496$ Å and $c=8.341$ Å (Ref. 12). Atomic spheres radii were chosen as $R(\text{Gd})=3.72$ a.u. and $R(\text{Fe})=2.66$ a.u. for the hexagonal structure, and $R(\text{Gd})=2.86$ a.u.¹⁵

and $R(\text{Fe})=2.62$ a.u. – for the rhombohedral structure.¹² Orbital basis contained $6s$, $6p$, $5d$, and $4f$ muffin-tin orbitals for Gd and $4s$, $4p$, and $3d$ for Fe sites. Integration over the first Brillouin zone was performed using 32 irreducible \mathbf{k} -points ($6 \times 6 \times 6 = 216$ is a total number of \mathbf{k} -points). Empty atomic spheres without nuclear charge were inserted in the case of the hexagonal structure to fill the interstitial regions.

In the LSDA+ U method Coulomb interaction for Gd $4f$ -orbitals was taken into account via parameters of direct U and exchange J Coulomb interactions of the $4f$ -electrons in Gd. For $\text{Gd}_2\text{Fe}_{17}$ in both structures the calculations of these parameters in the constrained LDA method¹⁷ resulted in $U_{\text{Gd}}=6.7$ eV and $J_{\text{Gd}}=0.7$ eV that is in agreement with the values for Gd metal.¹³

Local magnetic moments for various Fe and Gd sites obtained in the calculations are listed in Table I for both phases under consideration. Note that in qualitative discussions of magnetic properties of $R_2\text{Fe}_{17}$ especial attention is frequently paid to the iron ions in the dumbbell positions (Fe1 in our notations). From Table I one can see that magnetic moments of the Fe1 ions for the hexagonal structure are larger than for the rhombohedral one. However, total magnetic moment $M(\Sigma\text{Fe})$ value of the iron subsystem in the rhombohedral phase is larger ($M_{rh}(\Sigma\text{Fe})=38.04 \mu_B/\text{f.u.}$ vs. $M_{hex}(\Sigma\text{Fe})=36.54 \mu_B/\text{f.u.}$). Experimental value of total Fe ions magnetic moment for the mixture of two phases is $36.9 \mu_B/\text{f.u.}$.²⁶ Magnetic moments of the Gd ions in both calculations are antiparallel to the iron magnetic moments, so that the total magnetic moments are $M_{rh}(\Sigma\text{Fe} + \text{Gd})=23.70 \mu_B/\text{f.u.}$ and $M_{hex}(\Sigma\text{Fe} + \text{Gd})=22.21 \mu_B/\text{f.u.}$, respectively. These values agree well with experimental ones $M_S^{rh}=21.5 \mu_B/\text{f.u.}$ ¹¹ and $M_S^{hex}=21.2 \mu_B/\text{f.u.}$,¹² correspondingly.

III. EXCHANGE INTERACTIONS

In the framework of spin-fluctuation theory of magnetism it was found^{20,21,22,23} that the magnetic behavior of transition metals can be described by the Heisenberg model with long-range exchange interactions between classical spin vectors, in general, their magnitudes are non-integer. For an intermetallic magnet with several types of magnetic moments a spin Hamiltonian of such a model can be written as

TABLE I: Calculated values of local magnetic moments for both rhombohedral and hexagonal phases of Gd₂Fe₁₇.

rhombohedral structure		hexagonal structure	
Site	$M(\mu_B)$	Site	$M(\mu_B)$
Gd(6c)	-7.17	Gd(2b)	-7.13
		Gd(2d)	-7.20
Fe(6c)=Fe1	2.19	Fe(4f)=Fe1	2.31
Fe(9d)=Fe2	2.26	Fe(6g)=Fe2	2.10
Fe(18f)=Fe3	2.17	Fe(12j)=Fe3	2.40
Fe(18h)=Fe4	2.31	Fe(12k)=Fe4	1.87

$$H = -\frac{1}{2} \sum_{a,b} \sum_{\mathbf{l}_a, \mathbf{n}_b, \mathbf{l}_a \neq \mathbf{n}_b} I_{ab}(\mathbf{l}_a - \mathbf{n}_b) \mathbf{S}_a(\mathbf{l}_a) \mathbf{S}_b(\mathbf{n}_b), \quad (1)$$

where a and b are types of magnetic ions (e.g. a =Fe1, Fe2, Fe3, and Fe4), \mathbf{l}_a – radius vector of a magnetic ion of the a type, $\mathbf{S}_a(\mathbf{l}_a)$ – classical spin vector with the magnitude S_a , corresponding to magnetic moment $\mu_a = g\mu_B S_a$, and $I_{ab}(\mathbf{l}_a - \mathbf{n}_b)$ is an exchange parameter between ions of the types a and b with the distance $\mathbf{l}_a - \mathbf{n}_b$ between the ions.

Later an ab-initio method to calculate the exchange interaction parameters between different lattice sites for the classical Heisenberg model at $T=0$ was proposed.²⁴ In that scheme the exchange interaction parameters are determined calculating the second-order derivative of the total energy at $T=0$ with respect to small deviations of magnetic moments of the corresponding lattice sites from collinear magnetic configuration. This method was used in the present work to calculate the exchange interaction parameters I_{ab} (a, b =Fe1, Fe2, Fe3, Fe4) in the iron sublattice of both structures of Gd₂Fe₁₇.

First note that in Ref. 24 the energy of exchange interaction between different sites of the magnetic lattice is presented in the form $E_{ex}(\mathbf{l} - \mathbf{n}) = -2J_{ab}^L(\mathbf{l}_a - \mathbf{n}_b) \mathbf{e}_a(\mathbf{l}_a) \mathbf{e}_b(\mathbf{n}_b)$ as an exchange between two classical unit spin vectors $\mathbf{e}_a(\mathbf{l}_a) = (\sin\phi_a(\mathbf{l}_a)\sin\Theta_a(\mathbf{l}_a), \cos\phi_a(\mathbf{l}_a)\sin\Theta_a(\mathbf{l}_a), \cos\Theta_a(\mathbf{l}_a))$ and $\mathbf{e}_b(\mathbf{n}_b)$ regardless of the magnitude of the magnetic moments μ_a and μ_b at the sites \mathbf{l}_a and \mathbf{n}_b under consideration. Since the classical spin vector $\mathbf{S}_a(\mathbf{l}_a)$ is equal to $\mathbf{S}_a(\mathbf{l}_a) = S_a \mathbf{e}_a(\mathbf{l}_a)$, hence the relation between the ex-

change parameters J_{ab}^L calculated using the method of Ref. 24 and the exchange parameters I_{ab} of the Hamiltonian (1) will be given as $2J_{ab}^L = I_{ab}S_aS_b$. Moreover, some authors²⁵ calculating exchange parameters for insulators prefer to write the energy of exchange interaction as $E_{ex}(\mathbf{l}-\mathbf{n}) = -J_{ab}^M(\mathbf{l}_a - \mathbf{n}_b)\mathbf{S}_a(\mathbf{l}_a)\mathbf{S}_b(\mathbf{n}_b)$ via the exchange parameters J_{ab}^M between classical spin vectors with the magnitude $S_a, S_b=1/2$. It is easy to demonstrate that if one uses the method of Ref. 25 to calculate J_{ab}^M , then our exchange parameters I_{ab} are related with J_{ab}^M via the equality $I_{ab} = J_{ab}^M/(4S_aS_b)$.

Generally, in the intermetallic compounds of the $R_2\text{Fe}_{17}$ type there are many types of exchange interaction: R - R , R - Fe , and Fe - Fe . The weakest interaction is an indirect interaction of the R - R type between the rare-earth ions, because even for the nearest rare-earth ions their wave functions practically do not overlap.

Exchange interaction R - Fe is also indirect since direct overlap of $4f$ orbitals of the R ions and $3d$ orbitals of the neighboring iron ion is absent, and only small overlap of a polarized $5d$ orbital of the rare-earth ion and $3d$ orbital of the iron ions is possible. Theoretical estimation of this interaction is still difficult, nevertheless, from some indirect experiments this interaction can be estimated as 10–30 meV.²⁶ The sign of the exchange interaction R - Fe defines the orientation of the magnetic moment on the rare-earth ion with respect to the magnetic moments of the iron sublattice that seriously affects the saturation moment. At the same time, the dominating contribution to free energy of the magnetic system is due to the interaction of the Fe - Fe type which defines in fact the value of the critical temperature T_C . Because the number of iron ions is 8.5 times greater than the number of R ions, and in the Fe subsystem – there is also direct exchange between the neighboring Fe ions and the overlapping $3d$ wave functions.

In such complicated crystal structures as $\text{Th}_2\text{Zn}_{17}$ and $\text{Th}_2\text{Ni}_{17}$ the nearest neighbors in different crystallographic directions are arranged at different distances. However, analyzing the nearest neighbors of magnetic ions of each type $\text{Fe}1$, $\text{Fe}2$, $\text{Fe}3$, and $\text{Fe}4$ in both structures, the following regularities can be found. If one considers a spherical layer with the radii from $r_1^{rh}=2.385 \text{ \AA} < r < r_2^{rh}=2.740 \text{ \AA}$ around a particular ion $\text{Fe}a$ ($a=1, 2, 3, 4$) in the rhombohedral structure, then all nearest magnetic neighbors will be within this coordination layer. Next is an empty spherical layer without ions $r_2^{rh}=2.740 \text{ \AA} < r < r_3^{rh}=4.044 \text{ \AA}$. The second spherical coordination layer will be at $4.044 \text{ \AA} < r_3^{rh} < 4.3 \text{ \AA}$.²⁷ The only exception from this regularity is the $\text{Fe}3$ class with the nearest neighbor $\text{Fe}3$ -type ion at $r_{in}^{rh}=3.563 \text{ \AA}$

between the first and second coordination layers. It is typical that the atomic sphere of the chosen (“central”) ion Fe_a ($a=1, 2, 3, 4$) and atomic spheres of nearest Fe_a ($a=1, 2, 3, 4$) ions overlap. Therefore the direct exchange gives a dominant contribution in exchange parameters of the nearest neighbor Fe ions.

Similarly, in the hexagonal structure of Gd_2Fe_{17} each ion Fe_a ($a=1, 2, 3, 4$) can be surrounded by the first spherical coordination layer with the radii $r_1^{hex}=2.399 \text{ \AA} < r < r_2^{hex}=2.735 \text{ \AA}$, then an empty spherical layer without ions with $r_2^{hex}=2.735 \text{ \AA} < r < r_3^{hex}=4.108 \text{ \AA}$, and the second spherical coordination layer with $4.108 \text{ \AA} \leq r \leq 4.3 \text{ \AA}$. In exactly the same way the Fe3 ions violate this regulation, since these ions have a neighbor at $r_{in}^{hex}=3.605 \text{ \AA}$ between the first and second coordination layers.

The results for the exchange interaction parameters $I_{ab}(\mathbf{l}_a - \mathbf{n}_b)$ between different pairs of iron ions (in units of K) are presented in Tables II–V. In Table II the parameters of exchange interaction (in the descending order of absolute values) between the central ion Fe_a ($a=1, 2, 3, 4$) and ions of different types from the first coordination layer are presented. Here $I_{34}(1)$ stands for the value of the exchange parameter between ions Fe3 and Fe4 at the nearest distance between these ions (index 1 in the brackets), then $I_{34}(2)$ denotes the value of the exchange parameter between ions Fe3 and Fe4 at the second-order distance between these ions (index 2). Moreover, in Table II the number of neighbors $Z_{ab}(r)$ for a given distance are presented. This value gives the number of neighbors for the central ion Fe_a at the distance r . One should note that in our crystal structures $Z_{ab}(r) \neq Z_{ba}(r)$ (e.g. $Z_{13}(1)=6$ and $Z_{31}(r)=2$, i.e. the Fe1 ion has 6 neighbors of Fe3 at $r_{13}(1)=2.735 \text{ \AA}$, whereas the Fe3 ion has only 2 Fe1 ions at the same distance $r_{31}(1)=2.735 \text{ \AA}$).

It is observed that for the hexagonal Gd_2Fe_{17} all exchange parameters for each Fe_a ion with other ions Fe from the first spherical layer are positive i.e. ferromagnetic. Surprisingly, the exchange interaction parameter between the Fe4 ions within the corrugated hexagon plane $I_{44}(1)=218.5 \text{ K}$ is just a little less than the exchange parameter $I_{11}(1)=238.8 \text{ K}$ between the Fe1 ions at the dumbbell positions. Also, one should note that there is no simple dependence between the distance of the interacting Fe ions and the value of exchange interaction. For example, in the pair Fe3-Fe3 at the second-order distance $r_{33}(2)=2.512 \text{ \AA}$ the exchange interaction parameter is equal to $I_{33}(2)=123.4 \text{ K}$, whereas in the same plane of hexagons Fe3 in the pair Fe3-Fe3 at the distance $r_{33}(2)=2.403 \text{ \AA}$ the exchange interaction parameter is smaller, namely $I_{33}(1)=80.4 \text{ K}$.

TABLE II: Parameters of exchange in the hexagonal structure of $\text{Gd}_2\text{Fe}_{17}$ for the ions of the first coordination sphere.

N	Exchange (K)	Distance (\AA)	Number of neighbors	Type
1	$I_{11}(1)=238.8$	$r_{11}(1)=2.400$	$z_{11}(1)=1$	Fe1 (dumbbell) - Fe1 (dumbbell)
2	$I_{44}(1)=218.5$	$r_{44}(1)=2.477$	$z_{44}(1)=2$	Fe4 (corrugated plane) - Fe4 (corrugated plane)
3	$I_{34}(1)=136.1$	$r_{34}(1)=2.511$	$z_{34}(1)=z_{43}(1)=2$	Fe3 (dumbbell) - Fe4 (dumbbell)
4	$I_{33}(2)=123.4$	$r_{33}(2)=2.512$	$z_{33}(2)=1$	Fe3 - Fe3
5	$I_{24}(1)=101.9$	$r_{24}(1)=2.459$	$z_{24}(1)=4, z_{42}(1)=2$	Fe2 - Fe4 (corrugated layer)
6	$I_{23}(1)=90.7$	$r_{23}(1)=2.464$	$z_{23}(1)=4, z_{32}(1)=2$	Fe2 (corrugated layer) - Fe3 (upper and lower layer)
7	$I_{13}(1)=90.5$	$r_{13}(1)=2.735$	$z_{13}(1)=6, z_{31}(1)=2$	Fe1 (dumbbell) or Fe3 - Fe1 (dumbbell above and below)
8	$I_{33}(1)=80.4$	$r_{33}(1)=2.403$	$z_{33}(1)=1$	Fe3 - Fe3
9	$I_{14}(1)=72.0$	$r_{14}(1)=2.653$	$z_{14}(1)=3, z_{41}(1)=1$	Fe1 (dumbbell) - Fe4 (nearest corrugated layer)
10	$I_{12}(1)=69.3$	$r_{12}(1)=2.616$	$z_{12}(1)=3, z_{21}(1)=2$	Fe1 (dumbbell) - Fe2 (nearest corrugated layer)
11	$I_{34}(2)=61.3$	$r_{34}(2)=2.672$	$z_{34}(2)=z_{43}(2)=2$	Fe3 - Fe4 (corrugated layer above and below)

The method of exchange interaction parameters calculation employed here works in such a way that does not distinguish different mechanisms. There are several exchange interaction scenario super exchange, double exchange, direct exchange and RKKY one. First two require nonmagnetic interstitial ions in the system, that is not the case here. Thus only last two mechanisms are applicable. Direct exchange mostly come from orbitals overlap. One can suppose that absence of straightforward correlations between exchange parameter values and corresponding interatomic distances for the first coordination sphere for different crystallographic directions is connected with the way how Fe-3d orbitals overlap in these directions. However classification of the orbitals for these quite complicated crystal structures is highly non-trivial task which we postpone for future investigations. In addition some anisotropy in the first coordination sphere of exchange parameters might come from RKKY interaction since the Fermi surface of these compounds is rather complicated. For the second coordination sphere RKKY interaction is dominant but still might be highly anisotropic because of direction dependence of \mathbf{k}_F .

In Table III the parameters of exchange interaction of the ion Fe_a ($a=1, 2, 3, 4$) with some ions from the second-order coordination layer with $r > r_3^{hex}=4.108 \text{ \AA}$, as well as

TABLE III: Parameters of indirect exchange in the hexagonal structure of $\text{Gd}_2\text{Fe}_{17}$ for ions of the second coordination sphere.

N	Exchange (K)	Distance (\AA)	Number of neighbors	Type
1	$I_{34}(3)=14.0$	$r_{34}(3)=4.135$	$z_{34}(3)=2, z_{43}(3)=2$	Fe3 - Fe4
2	$I_{34}(4)=5.6$	$r_{34}(4)=4.172$	$z_{34}(4)=2, z_{43}(4)=2$	Fe3 - Fe4
3	$I_{14}(2)=4.2$	$r_{14}(2)=4.201$	$z_{14}(2)=3, z_{41}(2)=1$	Fe1 (dumbbell) - Fe4 (corrugated layer)
4	$I_{23}(2)=-7.9$	$r_{23}(2)=4.038$	$z_{23}(2)=4, z_{32}(2)=2$	Fe3 - Fe2 (corrugated layer)
5	$I_{33}(3)=-10.7$	$r_{33}(3)=3.605$	$z_{33}(3)=1$	Fe3 - Fe3
6	$I_{33}(5)=-13.2$	$r_{33}(3)=4.257$	$z_{33}(5)=2$	Fe3 - Fe3
7	$I_{12}(2)=-14.6$	$r_{12}(2)=4.108$	$z_{12}(2)=3, z_{21}(2)=2$	Fe1 (dumbbell) - Fe2 (corrugated layer)
8	$I_{34}(5)=-16.3$	$r_{34}(5)=4.220$	$z_{34}(5)=2, z_{43}(5)=2$	Fe3 - Fe4 (corrugated layer)
9	$I_{22}(2)=-18.1$	$r_{22}(2)=4.260$	$z_{22}(2)=4$	Fe2 (corrugated layer) - Fe2 (corrugated layer)
10	$I_{33}(4)=-29.0$	$r_{33}(4)=4.239$	$z_{33}(4)=2$	Fe3 - Fe3 (layer above and below)
11	$I_{22}(1)=-111.1$	$r_{22}(1)=4.182$	$z_{22}(1)=2$	Fe2 - Fe2 (layer above and below)

the exchange parameters $I_{33}(3)$ for $r_{33}(3) = r_{in}^{hex}=3.605 \text{ \AA}$ in a Fe3-Fe3 pair at the third-order distance, in the hexagonal structure of $\text{Gd}_2\text{Fe}_{17}$ are presented. At these distances the exchange parameters are mostly negative, antiferromagnetic, and are usually an order of magnitude less than the exchange parameters with the ions of the first-order coordination layer. At the same time, a sufficiently strong antiferromagnetic exchange $I_{22}(1)=-111.1 \text{ K}$ in both pairs of the nearest neighbors Fe2-Fe2 from the neighboring corrugated planes is present.

In Table IV the parameters of exchange interaction of the ion Fe_a ($a=1, 2, 3, 4$) with the ions from the first coordination layer, as well as the exchange parameters $I_{33}(2)$ with the Fe3 ions located between the first and second layers, in the rhombohedral structure of $\text{Gd}_2\text{Fe}_{17}$ are shown. Transferring from the hexagonal to the more compact rhombohedral structure of $\text{Gd}_2\text{Fe}_{17}$, the distance in a dumbbell Fe1-Fe1 decreases from $r_{11}^{hex}(1)=2.400 \text{ \AA}$ to $r_{11}^{rh}(1)=2.385 \text{ \AA}$. Where from the exchange parameter $I_{11}(1)$ increases from $I_{11}^{hex}(1)=238.8 \text{ K}$ to $I_{11}^{rh}(1)=287.5 \text{ K}$. However, the second largest interaction $I_{44}(1)$ in the corrugated hexagon plane and the third largest interaction $I_{34}(1)$ between the layers of Fe3 and Fe4 are smaller in the rhombohedral structure of $\text{Gd}_2\text{Fe}_{17}$: $I_{44}^{hex}(1)=218.5 \text{ K}$ vs. $I_{44}^{rh}(1)=182.2 \text{ K}$.

TABLE IV: Parameters of exchange in the rhombohedral structure of $\text{Gd}_2\text{Fe}_{17}$ for the ions of the first coordination sphere and indirect exchange $I_{33}(2)$.

N	Exchange (K)	Distance (\AA)	Number of neighbors	Type
1	$I_{11}(1)=287.5$	$r_{11}(1)=2.385$	$z_{11}(1)=1$	Fe1 (dumbbell) - Fe1 (dumbbell)
2	$I_{44}(1)=182.2$	$r_{44}(1)=2.490$	$z_{44}(1)=2$	Fe4 (corrugated plane) - Fe4 (corrugated plane)
3	$I_{34}(1)=125.9$	$r_{34}(1)=2.551$	$z_{34}(1)=z_{43}(1)=2$	Fe3 - Fe4 (corrugated plane)
4	$I_{33}(2)=121.9$	$r_{33}(2)=3.563$	$z_{33}(2)=1$	Fe3 - Fe3
5	$I_{24}(1)=121.0$	$r_{24}(1)=2.448$	$z_{24}(1)=4, z_{42}(1)=2$	Fe2 (corrugated layer) - Fe4 (corrugated layer)
6	$I_{34}(2)=105.7$	$r_{34}(2)=2.613$	$z_{34}(2)=z_{43}(2)=2$	Fe3 - Fe4 (corrugated layer)
7	$I_{14}(1)=88.8$	$r_{14}(1)=2.639$	$z_{14}(1)=3, z_{41}(1)=1$	Fe1 (dumbbell) - Fe4 (corrugated layer)
8	$I_{23}(1)=87.1$	$r_{23}(1)=2.423$	$z_{23}(1)=4, z_{32}(1)=2$	Fe3 - Fe2 (corrugated layer)
9	$I_{12}(1)=83.6$	$r_{12}(1)=2.602$	$z_{12}(1)=3, z_{21}(1)=2$	Fe1 (dumbbell) - Fe2 (corrugated layer)
10	$I_{13}(1)=74.1$	$r_{13}(1)=2.740$	$z_{13}(1)=6, z_{31}(1)=2$	Fe1 (dumbbell) - Fe3
11	$I_{33}(1)=-36.5$	$r_{33}(1)=2.466$	$z_{33}(1)=2$	Fe3 - Fe3

While $r_{44}^{hex}(1)=2.478 \text{ \AA}$ is smaller than $r_{44}^{rh}(1)=2.490 \text{ \AA}$, and $r_{34}^{hex}(1)=2.511 \text{ \AA}$ smaller than $r_{34}^{rh}(1)=2.549 \text{ \AA}$ $I_{34}^{hex}(1)=136.1 \text{ K}$ exceeds $I_{34}^{rh}(1)=125.9 \text{ K}$. Also, in the rhombohedral structure one antiferromagnetic exchange (with negative value) appears since $I_{33}^{hex}(1)=80.4 \text{ K}$ in the hexagonal structure becomes $I_{33}^{rh}(1)=-36.5 \text{ K}$ in the rhombohedral one, whereas $r_{33}^{hex}(1)=2.403 \text{ \AA}$ will be enhanced to $r_{33}^{rh}(1)=2.466 \text{ \AA}$. Similar results are obtained for rhombohedral Y_2Fe_{17} in Ref. 28.

Finally, Table V contains exchange parameters for the second coordination sphere of rhombohedral $\text{Gd}_2\text{Fe}_{17}$. As in the case of hexagonal phase most of them are antiferromagnetic and considerably weaker in comparison with the first coordination layer.

From these data it is clear that a decrease of the distance in a pair of interacting ions in the first coordination sphere results in an increase of the ferromagnetic exchange parameter. But since the distance in the basic structural elements changes in opposite way from the hexagonal to rhombohedral structure (the distance decreases in the dumbbells, and mostly increases in the hexagons), then it is reasonable to use the Curie point T_C to estimate collective effect of these changes in the distances and corresponding exchange parameters transferring from one structure of $\text{Gd}_2\text{Fe}_{17}$ to another. Let us use Weiss mean-field theory

TABLE V: Parameters of exchange in the rhombohedral structure of Gd₂Fe₁₇ for the ions of the second coordination sphere.

N	Exchange (K)	Distance (Å)	Number of neighbors	Type
1	$I_{14}(2)=12.3$	$r_{14}(2)=4.206$	$z_{14}(2)=3$	Fe1 (dumbbell) - Fe4 (corrugated layer)
2	$I_{23}(2)=1.6$	$r_{23}(2)=4.063$	$z_{23}(2)=4, z_{32}(2)=2$	Fe2 (corrugated layer)- Fe3
3	$I_{34}(3)=-1.2$	$r_{34}(3)=4.132$	$z_{34}(3)=z_{43}(2)=2$	Fe3 - Fe4 (corrugated layer)
4	$I_{12}(2)=-3.6$	$r_{12}(2)=4.095$	$z_{12}(2)=3, z_{21}(2)=2$	Fe1 (dumbbell) - Fe2 (corrugated layer)
5	$I_{34}(5)=-5.0$	$r_{34}(5)=4.190$	$z_{34}(5)=z_{43}(5)=2$	Fe3 - Fe4 (corrugated layer)
6	$I_{13}(2)=-15.2$	$r_{13}(2)=4.237$	$z_{13}(2)=6, z_{31}(2)=2$	Fe1 (dumbbell) - Fe3
7	$I_{34}(4)=-16.4$	$r_{34}(4)=4.171$	$z_{34}(4)=z_{43}(4)=2$	Fe3 - Fe4 (corrugated layer)
8	$I_{33}(3)=-20.4$	$r_{33}(3)=4.192$	$z_{33}(3)=2$	Fe3 - Fe3
9	$I_{44}(2)=-36.7$	$r_{44}(2)=3.841$	$z_{44}(2)=1$	Fe4(corrugated layer) - Fe4 (corrugated layer)
10	$I_{44}(3)=-57.5$	$r_{44}(3)=4.236$	$z_{44}(4)=2$	Fe4(corrugated layer) - Fe4 (corrugated layer)

taking into account only the Fe-Fe exchange interactions.

Within the Weiss mean-field theory the Hamiltonian (1) can be written as

$$H^{MF} = \frac{1}{2} \sum_{a,b} \sum_{\mathbf{l}_a, \Delta_b} I_{ab}(\Delta_b) \langle S_a^Z(\mathbf{l}_a) \rangle \langle S_b^Z(\mathbf{l}_a + \Delta_{ab}) \rangle - \sum_a \sum_{\mathbf{l}_a} h_a(\mathbf{l}_a) S_a^Z(\mathbf{l}_a), \quad (2)$$

where $\Delta_{ab} = \mathbf{n}_b - \mathbf{l}_a$, and molecular field $h_a(\mathbf{l}_a)$ for spin $\mathbf{S}_a(\mathbf{l}_a)$ can be presented as

$$h_a(\mathbf{l}_a) = \sum_{b, \Delta_{ab}} I_{ab}(\Delta_{ab}) \langle S_b^Z(\mathbf{l}_a + \Delta_{ab}) \rangle = \sum_{b, |\Delta_{ab}|} I_{ab}(|\Delta_{ab}|) z_{ab}(|\Delta_{ab}|) \sigma_b. \quad (3)$$

Here $\sigma_b = \langle S_b^Z(\mathbf{l}_a + \Delta_{ab}) \rangle$ denotes the thermodynamic average of z -projection of classical spin for the ion Fe b ($b=1, 2, 3, 4$). $z_{ab}(|\Delta_{ab}|)$ is the number of Fe b neighbors at the distance $|\Delta_{ab}|$ from the central ion Fe a .

Calculating the average value σ_a in a field h_a , one obtains a set of self-consistent equations for σ_a ($a=1, 2, 3, 4$):

$$\sigma_a = S_a L\left(\frac{h_a S_a}{k_B T}\right) = S_a \left[\coth\left(\frac{h_a S_a}{k_B T}\right) - \frac{k_B T}{h_a S_a} \right] \quad (4)$$

($L(x) = \coth(x) - 1/x$ - Langevin function). Linearizing the set Eq. (4) with respect to

small σ_a , one obtains a set of linear equations for T_C :

$$k_B T_C \sigma_a = \frac{S_a^2}{3} \sum_b \sum_{|\Delta_{ab}|} I_{ab}(|\Delta_{ab}|) z_{ab}(|\Delta_{ab}|) \sigma_b. \quad (5)$$

Let us solve the set of equations (5) for the rhombohedral and hexagonal structures of $\text{Gd}_2\text{Fe}_{17}$ restricting ourselves by using $I_{ab}(|\Delta_{ab}|)$ and $z_{ab}(|\Delta_{ab}|)$ as the parameters of direct exchange and number of neighbors in the first coordination layer (Tables IV and II). Upon these assumptions the estimations for the Curie point for exchanges only from the first coordination layer are $T_C^{rh}=429$ K and $T_C^{hex}=402$ K. These estimations are below the experimental values $T_C^{rh}=475$ K (Ref. 11) and $T_C^{hex}=466$ K (Ref. 12). Such a situation is typical for estimations of T_C for ferromagnetic metals in the framework of the molecular field approximation (c.f. for instance, estimations for Fe, Co and Ni²⁹). At the same time these theoretical values grasp a trend of the Curie temperature growth in transferring from the rhombohedral to the hexagonal structures in $\text{Gd}_2\text{Fe}_{17}$ what takes place in experiments Refs. 11,12. Here we can address also a question how T_C changes in case second coordination sphere is taken into account. As shown above in Tables II-V next nearest exchanges are predominantly AFM-like but are weaker. Thus one should expect a bit of lowering of resulting T_C . Indeed, we found $T_C^{rh}(1st+2nd)=378$ K and $T_C^{hex}(1st+2nd)=353$ K. Nevertheless a trend of the Curie temperature growth from the rhombohedral to the hexagonal structure is still observed.

But comparing these values one should keep in mind several reasons why the calculated results of T_C cannot *precisely* fit the experiment.

Firstly, in accord with spin-fluctuation theory of magnetism approximating magnetic excitations in metals with the classical Heisenberg Hamiltonian, all exchange interactions in metals are long-range, relatively slowly decaying, and sign oscillating (similar to Ruderman-Kittel interaction).^{21,23} This conclusion also follows from our results for the hexagonal structure of $\text{Gd}_2\text{Fe}_{17}$, see Table III (for the rhombohedral structure see Table V), where the exchange interaction of the Fe ions with the neighbors of the second-order coordination layer mostly change their sign and become negative, antiferromagnetic. Exact account of these oscillating interactions requires either exact functional form of the exchange distance dependence for a particular pair of ions (e.g., Fe1-Fe3), or calculation of the exchange parameters for such a pair on the scale of a few oscillations. At the moment the method of Ref. 24 allows one to calculate the exchange parameters, but it is not clear how to present an

explicit functional dependence of the exchange on distance. Nevertheless, in principle in this method one can calculate exchange parameters on the scale of a few oscillations, but for a metallic magnet with several types of magnetic moments and complicated crystal structure it is a cumbersome problem.

Secondly, also according to spin-fluctuation theory in metals,²¹ the exchange parameters of the classical Heisenberg Hamiltonian in the general case are temperature dependent. For this reason, the exchange parameters at $T=0$ and $T=T_C$ differ, whereas in our calculations we estimated T_C from the exchange parameters calculated using the $T=0$ method of Ref. 24.

Thirdly, an obvious limitation of such calculations is the Weiss mean-field theory, restricted in its accuracy.

Before we summarize let us also compare magnetic properties of elemental *bcc* Fe to ones averaged over first coordination sphere of Fe ions of hexagonal $\text{Gd}_2\text{Fe}_{17}$. First of all value of nearest neighbor exchange interaction of *bcc* Fe (393.2 K, Ref. 19; 373.6 K, Ref. 30) is four times larger than the above mentioned averaged value of $\text{Gd}_2\text{Fe}_{17}$ (99.6 K, Ref. 31). It can be understood from difference of the nearest neighbor distance of *bcc* Fe (2.482 Å) and averaged distance of $\text{Gd}_2\text{Fe}_{17}$ (2.574 Å, Ref. 32). Thus hexagonal $\text{Gd}_2\text{Fe}_{17}$ has more loose-packed crystal structure than *bcc* Fe. This more loose-packed crystal structure also leads to a smaller saturation magnetization at $T=0$ of Fe ion sublattice in hexagonal $\text{Gd}_2\text{Fe}_{17}$ (1299 G, Ref. 34) in contrast to *bcc* Fe (1740 G, Ref. 33). It becomes even more clear since values of *bcc* Fe local magnetic moment ($2.2 \mu_B$) is almost equal to one averaged over all crystallographic positions for hexagonal $\text{Gd}_2\text{Fe}_{17}$ ($2.15 \mu_B$). Similar results can be obtained for rhombohedral phase of $\text{Gd}_2\text{Fe}_{17}$.

IV. CONCLUSION

In this work we calculate from first principles electronic structure and values of exchange interaction parameters of the Fe ions sublattice for the hexagonal and rhombohedral phases of intermetallic compound $\text{Gd}_2\text{Fe}_{17}$ within first and second coordination spheres. Based on the values of exchange interaction parameters Curie temperatures T_C were also calculated. Obtained theoretical Curie temperatures $T_C^{rh}=429$ K and $T_C^{hex}=402$ K are found to be slightly below the experimental values $T_C^{rh}=475$ K¹¹ and $T_C^{hex}=466$ K¹². However the

tendency of T_C^{rh} to be higher than T_C^{hex} is well reproduced. The same is found for the case if second coordination sphere is taken into account. Corresponding Curie temperatures are $T_C^{rh}(1st+2nd)=378$ K and $T_C^{hex}(1st+2nd)=353$ K.

Beside that from our calculations we observe that for the first coordination sphere exchange between different types of Fe ions is ferromagnetic (with only one exception for rhombohedral phase). At the same time exchange for next nearest neighbors is mostly antiferromagnetic one. Latter one is consistent with RKKY exchange picture (exchange sign depends on pair bond length).^{20,21,22,23} However such competition only is not enough to decrease significantly Curie temperature T_C of R_2Fe_{17} as proposed if Ref. 3. Also it was reported before that exchange value between Fe in dumbbell positions is the determining factor for the T_C value²⁸. However in this paper we showed that there are several exchange interactions almost of the same strength as dumbbell one, e.g. I_{44} (see Tab. II).

Let us also roughly analyze values of exchange interactions in terms of crystal structure. Collecting data from Tables II-V one can observe for both phases analogous tendency. Exchanges within any layer are weaker than interlayer ones. Exceptional is only Fe2 ion surrounded with four Fe4 ions with exchange $I_{24}(1)$. Anisotropy of direct exchange interaction parameters in the first coordination sphere comes from Fe-3d orbitals overlap anisotropy. On top of that RKKY exchange gives slight modulations in the first coordination sphere because of complexity of the Fermi surface of the compounds. For the second coordination sphere RKKY is main contribution to exchange interaction but for the reason mentioned above is also highly anisotropic.

After all we propose another one observation to explain relatively low T_C of R_2Fe_{17} series. To this end we compare magnetic properties of Fe ion sublattice of hexagonal Gd_2Fe_{17} to elemental *bcc* Fe. There are two ingredients influencing T_C value: local magnetic moment values and exchange interaction values. Despite the fact that for both hexagonal Gd_2Fe_{17} and *bcc* Fe local magnetic moments of Fe ion are almost identical, exchange interaction values of *bcc* Fe is four times stronger than for hexagonal Gd_2Fe_{17} ³¹. It comes from more dense packing of Fe ions of *bcc* Fe compared to hexagonal Gd_2Fe_{17} ³². The same arguments support lower saturation magnetization value for Gd_2Fe_{17} . Thus even for highest T_C compound Gd_2Fe_{17} of R_2Fe_{17} series magnetic properties are found to be inferior to ones of *bcc* Fe.

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- ³² Averaged over first coordination sphere Fe-Fe distance for hexagonal Gd₂Fe₁₇ is computed as

$$\bar{r}^{hex} = \frac{r_{11}(1)z_{11}(1)+r_{12}(4)z_{12}(1)+\dots+r_{44}(4)z_{44}(1)}{z_{11}(1)+z_{12}(1)+\dots+z_{44}(1)} = 2.574 \text{ \AA}, \text{ where } r_{ab} \text{ and } z_{ab} \text{ are taken from Tab. II.}$$

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³⁴ To get saturation magnetization at $T=0$ of Fe ion sublattice in hexagonal $\text{Gd}_2\text{Fe}_{17}$ we took magnetic moment per formula unit $M(\Sigma\text{Fe})=36.54 \mu_B$ and unitary cell volume $\Omega=521.4 \times 10^{-24} \text{ cm}^3$ (Ref. 12).

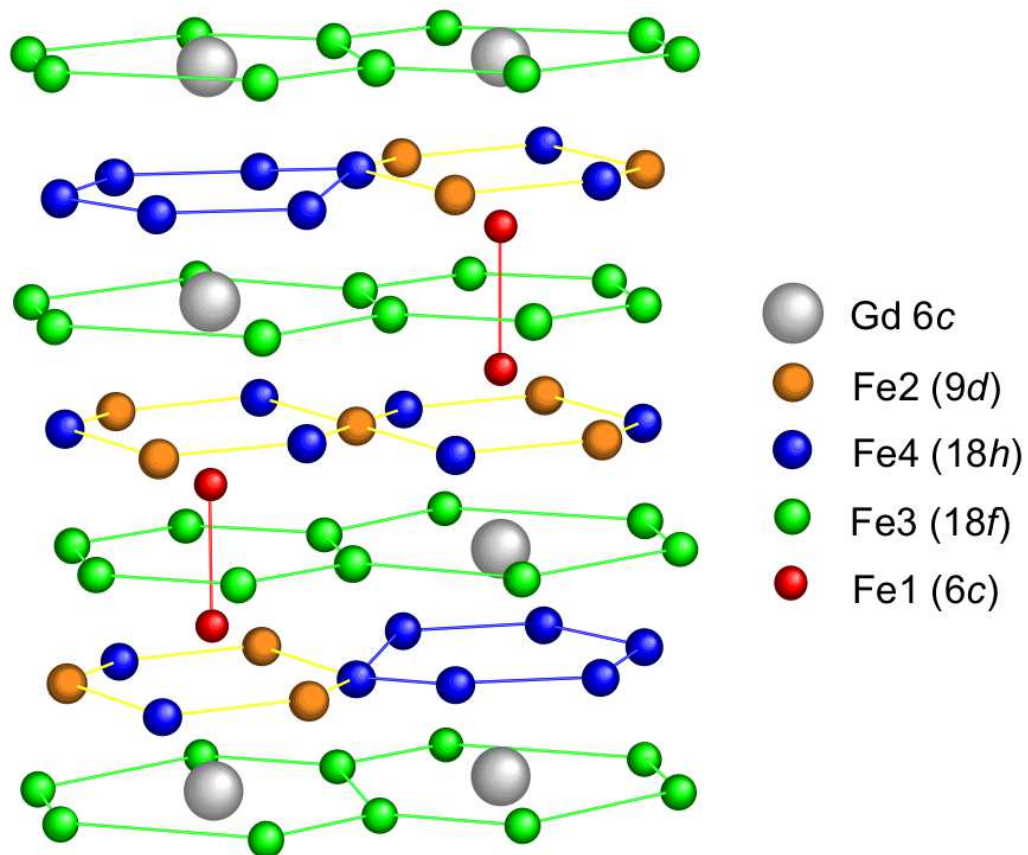


FIG. 1: (Color online) Rhombohedral Th_2Zn_{17} -type structure of Gd_2Fe_{17} .

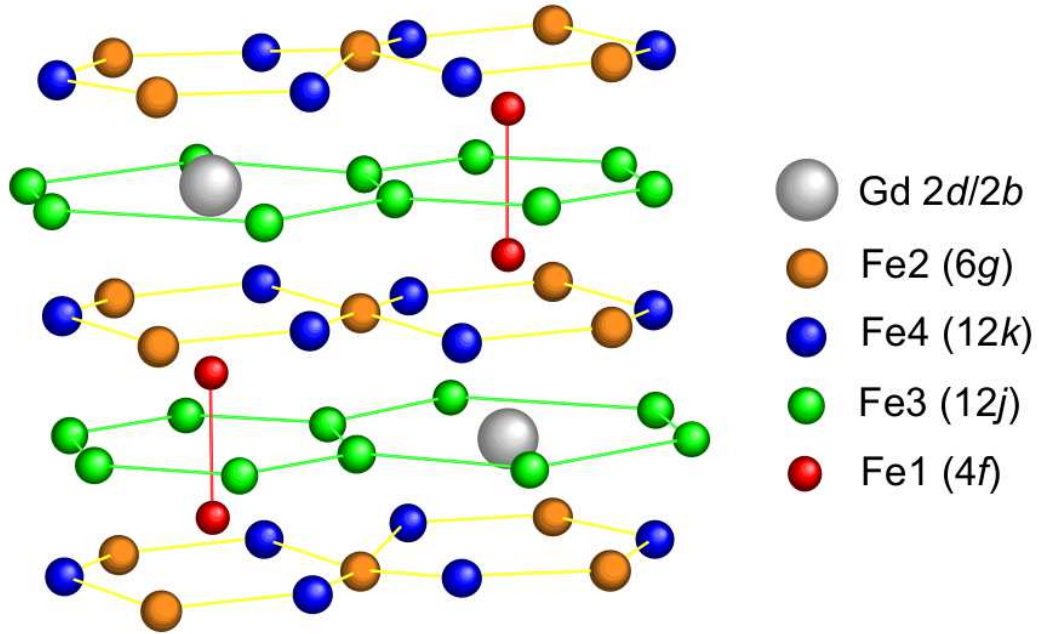


FIG. 2: (Color online) Hexagonal Th_2Ni_{17} -type structure of $\text{Gd}_2\text{Fe}_{17}$.