Физика

DOI: 10.14529/mmph250305

COMPUTER MODELING OF MAGNETIC PROPERTIES OF DISORDERED BCC PHASE OF $Fe_{100-X}Me_X$ ALLOYS (Me = AL, GA, GE)

M.A. Zagrebin[1], I.A. Markovich[2], A.S. Kuznetsov[1], M.V. Matyunina[1], A.V. Butakov[1]

[1] *Chelyabinsk State University, Chelyabinsk, Russian Federation*

[2] *South Ural State University, Chelyabinsk, Russian Federation*

E-mail: miczag@mail.ru

Abstract. In this paper, within the framework of density functional theory for the disordered phase *A*2 of Fe-*Me* alloys (*Me* = Al, Ga, Ge) the magnetic exchange constants J_{ij} are calculated and the Curie temperatures T_C are estimated in dependence of the concentration of *Me* = Al, Ga, Ge (in the range of $0 \le x \le 14$ at. %) and the crystal lattice parameter (in the range of $2{,}7 \le a \le 3{,}0$ Å). The J_{ij} distribution obtained in the paper demonstrates nonlinear behavior. The highest ferromagnetic interaction in the first coordination sphere is ≈23 meV. In the third coordination sphere, antiferromagnetic exchange interaction is observed, which reaches a value of ≈ –2,5 meV. Magnetic transition temperatures calculated using the mean field approximation based on the experimental values and the a_0 parameters calculated within the density functional theory show the presence of a concentration range of $4 \le x \le 8$ at. % in which T_C increases. The cross-section of the calculated Curie temperature distribution shows that for all studied Fe-*Me* alloys with the lattice parameter a_0 = 2,94 Å, it is possible to construct a dependence $T_C(x)$ that is in quality agreement with the experimental one.

Keywords: Fe-based alloys; ab initio calculations; magnetic exchange interaction; Curie temperature.

Introduction

The scientific community's interest in the research and development of multifunctional iron-based materials is constantly growing. The demand for environmentally friendly materials makes these alloys especially attractive. The unique combination of mechanical, magnetic, and electrical characteristics of Fe-*Me* alloys (*Me* = Al, Ga, Ge) with high magnetostriction values in low magnetic fields [1, 2] is of particular interest for researchers and makes such alloys promising for the creation of sensors and actuators and other magnetomechanical devices. The ability to convert magnetic energy into mechanical energy and vice versa allows these alloys to be used in industry, power engineering, automotive engineering, and other areas. Thus, studies of Fe-*Me* alloys (*Me* = Al, Ga, and Ge) remain relevant both from the point of view of fundamental science and practical application. This is confirmed by the constant growth in the number of publications in this field.

Experimental studies show that addition of nonmagnetic elements such as aluminum, gallium, or germanium into α-Fe with a body-centered cubic (*bcc*) lattice allows for a significant increase in the magnitude of tetragonal magnetostriction in the resulting alloys compared to pure iron [2]. The phase diagrams of the $Fe_{100-x}Me_x$ systems (*Me* = Al, Ga, Ge) in the concentration range from 0 to 10 at. % reveal the presence of a disordered *bcc* structure *A*2 (symmetry group no. 229, *Im*-3*m*, with α-Fe as prototype). In this case, similar behavior of parameters such as tetragonal magnetostriction and the Curie temperature is observed. In the single-phase *A*2 region, a gradual decrease in Curie temperature T_C is observed, which becomes sharper during the formation of the $D0_3$ structure. This is accompanied by the appearance of a two-phase region, which affects the magnetic characteristics of the material [3].

The theoretical calculation of the transition temperature from ferromagnetic (FM) to paramagnetic (PM) state, presented in [4–7], showed an interesting feature of the obtained results. A complex approach using *ab initio* calculations and Monte Carlo modeling reveals a decreasing behavior of the $T_C(x)$

curve dependences in the $Fe_{100-x}Al_x$, $Fe_{100-x}Ga_x$, and $Fe_{100-x}Ge_x$ alloys only in the concentration range of $x > 12$ at. %. However, in the region of lower concentrations, the behavior of the curve cannot be reproduced, since studies show the opposite trend: the Curie temperature increases with a change in the concentration of *Me* = Al, Ga, Ge from zero to 12 at. %. The authors explain this behavior by an increase in the exchange interaction J_{ij} between iron atoms, as well as an increase in the magnetic moment of Fe atoms μ_{Fe}. It is important to note the observed correlation between the values of J_{ij} and μ_{Fe} and the lattice parameter: the larger the lattice parameter, the stronger the exchange interaction and the greater the magnetic moment per iron atom [5, 6]. Thus, the obtained results indicate a complex relationship between the structure, composition, and magnetic properties of $Fe_{100-x}Me_x$ alloys (*Me* = Al, Ga, Ge), which opens up new prospects for basic research into the mechanisms of forming magnetic properties in these materials.

In this paper, we analyze the influence of the crystal lattice parameter and the concentration of nonmagnetic atoms of *Me* = Al, Ga, Ge on the exchange interaction, as well as the Curie temperature of the *A*2 structure of $Fe_{100-x}Me_x$ alloys ($0 \le x \le 14$ at. %) using *ab initio* simulation.

1. Calculation details

To simulate the magnetic properties in the $Fe_{100-x}Me_x$ (*Me* = Al, Ga, Ge, $0 \le x \le 14$ at. %) system, we used the Korringa–Kohn–Rostoker Green's function method implemented in the SPRKKR software package (a Spin Polarized Relativistic Korringa–Kohn–Rostoker code) [8]. The fully disordered structure *A*2 was investigated in the work. For this phase, Fe and Me atoms are randomly distributed in the Wyckoff position 2*a*(0, 0, 0). To create non-stoichiometric compositions, we used the single-site coherent potential approximation (CPA). The use of CPA allows us to construct an averaged potential for a lattice site occupied by several types of atoms [8]. Note that this approximation successfully describes the properties of many compositionally disordered (non-stoichiometric) alloys. The crystal lattice parameter in the calculations was varied in the range of $2{,}7 \le a \le 3{,}0$ Å.

In the first stage, we performed calculations of the Heisenberg magnetic exchange constants J_{ij} in the formulation of A. Lichtenstein *et al.* [9]. The calculations included the use of the spin-polarized scalar-relativistic Dirac Hamiltonian with $l_{max} = 3$. To perform both self-consistent and J_{ij} calculations, 4 495 *k*-points were generated by a 57×57×57 *k*-grid. For the exchange-correlation potential, the generalized gradient approximation in the Perdew–Burke–Ernzerhof (PBE) formulation was used [10]. Obtained exchange coupling constants were used to estimate the Curie temperature T_C in the mean field approximation [11]. J_{ij} parameters in Curie, temperature estimation were taken into account up to the 49th coordination sphere and were limited to a value multiple of 6 lattice parameters.

2. Results and discussion

At the first stage, the magnetic exchange interaction parameters were calculated for the *A*2 structure of the $Fe_{98}Ga_2$ alloy with the experimental lattice value $a_0 = 2{,}87$ Å [12]. Fig. 1 shows the values of J_{ij} between Fe atoms depending on the distance between the atoms (in units of the crystal lattice parameter). The exchange interaction between pairs of Ga-Ga and Fe-Ga atoms does not exceed 0,1 meV and is excluded from consideration. In Fig. 1, J_{ij} exhibit oscillating damped behavior. The largest FM interaction is observed in the first coordination sphere of Fe atoms and is ≈ 22 meV. Let us consider how the values of J_{ij} change depending on the crystal lattice parameter and the concentration of *Me* = Al, Ga, and Ge atoms.

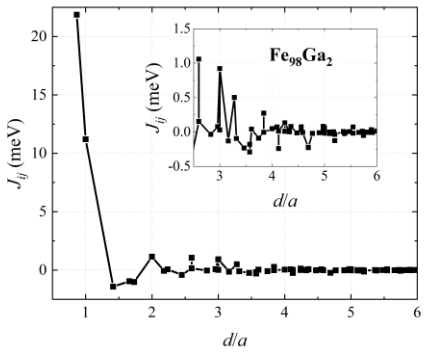

Fig. 1. Magnetic exchange interaction constants J_{ij} as a function of the distance (d/a) between the pairs of *i* and *j* atoms, calculated for the experimental lattice value. ($a_0 = 2{,}87$ Å) [11] in the *A*2 structure of the $Fe_{98}Ga_2$ alloy

Fig. 2 shows the distribution of the magnetic exchange interaction constants for the $Fe_{100-x}Al_x$ alloy series depending on the value of the crystal lattice and the concentration of Al atoms for the first three coordination spheres (Fig. 2(a) – at a distance of $\sqrt{3}/2\,a$, Fig. 2(b) – at a distance of a, and Fig. 2(c) – at a distance of $\sqrt{2}\,a$). The J_{ij} distribution has a non-linear behavior. Between the nearest Fe atoms (Fig. 2(a)), depending on the Al concentration, the change is no more than 5 meV, from ≈19 meV for pure Fe to ≈ 24 meV in the

case of $Fe_{86}Al_{14}$. Note that such an increase corresponds to the region of lattice parameters a = 2,85–2,86 Å, which is close to the experimental value. In the range of values $a \leq 2{,}76$ Å, J_{ij} demonstrate a weak dependence on the Al concentration, changing by 1 meV (≈20,5–≈ 21,5 meV), while in the range of $a \geq 2{,}92$ Å, the change in J_{ij} is greater than 3 meV (≈20 – ≈23,5 meV).

In the second coordination sphere (at a distance of a, Fig. 2(b)) the distribution of exchange parameters is different, and two regions can be distinguished in the distribution depending on the lattice parameter. In the first region with small values of the lattice parameters ($a \leq 2{,}82$ Å), the J_{ij} parameters change slightly with increasing Al concentration, increasing almost linearly with an increase in the lattice parameter at a fixed Al concentration in the alloy. In this region, the parameter values change from ≈4,5 to ≈10,5 meV. The second region in Fig. 2(b) is characterized by a decrease in magnetic exchange with an increase in the Al concentration at constant values of a and a fixed Al concentration in the alloy. In this region, the change in the parameters of the magnetic exchange interaction is observed from ≈8,0 to ≈14,0 meV.

In the case of interaction between Fe atoms located at a distance of $\sqrt{2}$ (Fig. 2(c), the third coordination sphere), a region of antiferromagnetic interaction is observed in the distribution. This region is observed for lattice parameters of $2{,}8 \leq a \leq 3{,}0$ Å and in the concentration range of $0 \leq x \leq 8$ at. %. In general, a weak (no more than 4 meV) change in the constants of magnetic exchange interaction in the third coordination sphere can be noted.

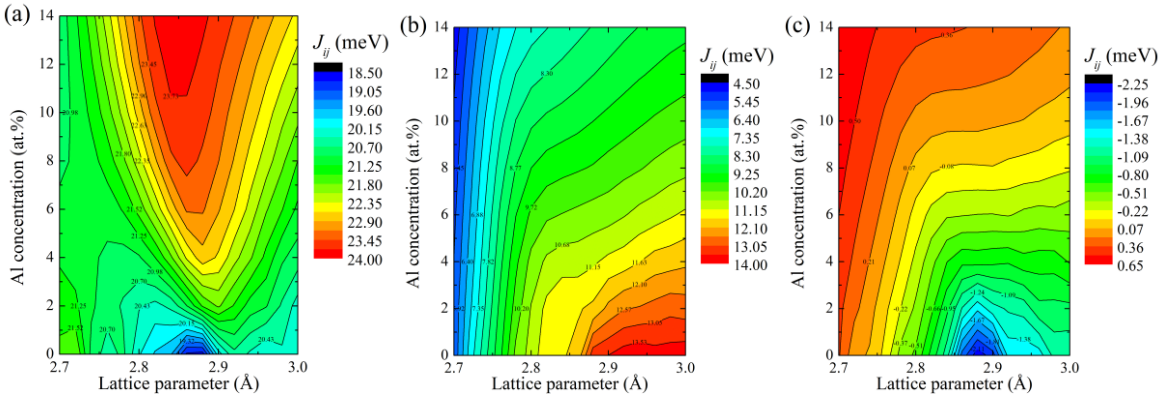

Fig. 2. Distribution of the magnetic exchange interaction constant of $Fe_{100-x}Al_x$ alloys between Fe atoms depending on the crystal lattice parameter *a* and the Al concentration *x* in (a) the first, (b) second, and (c) third coordination spheres

In Fe-Ga and Fe-Ge alloys, the behavior of the magnetic exchange interaction constants is similar. The difference lies in the magnitude of the parameters associated with the presence of *Me* = Al, Ga, Ge atoms in the alloys, which was shown earlier in our works [5–7, 13–17].

In [5–7, 13–17], the authors showed that when modeling using the Monte Carlo method, the calculated Curie temperature values depend significantly on J_{ij}'s value. Taking this fact into account, in the present work, we analyzed the influence of the value of the crystal lattice parameter and the concentration of nonmagnetic atoms in the $Fe_{100-x}Al_x$, $Fe_{100-x}Ga_x$ and $Fe_{100-x}Ge_x$ alloys on the Curie temperature. The values of T_C shown in Fig. 3 as a function of the crystal lattice parameter and the concentration of *Me* = Al, Ga, Ge atoms were obtained in the mean field approximation, which, as shown by the results of [4, 15], gives overestimated values compared to experimental values, but allows for a qualitative repetition of the experimentally observed trends [4, 18, 19].

Fig. 3 demonstrates that for all three systems: Fe-Al, Fe-Ga, and Fe-Ge, the T_C distributions are similar, and the main difference is observed in the range of lattice parameters from 2,9 to 3,0 Å. Up to lattice parameter values of $a \geq 2{,}94$ Å, Curie temperatures have a maximum in the range of *Me* = Al, Ga, Ge atomic concentrations from 0 to 2 at. %. This behavior does not coincide with the observed experimental concentration dependence of the Curie temperature, according to which the behavior of the $T_C(x)$ curve has a descending behavior when *Me* = Al, Ga, Ge atoms are added to pure iron [12, 20–22]. Note that in the case of the Fe-Ge alloy, a concentration of ≈ 4,5 at.% can be distinguished, where the second maximum is observed at a = 2,9 Å.

Fig. 3 shows the $T_C(x)$ cross-sections corresponding to the experimental values of the crystal lattice parameter [12, 20, 21] and the crystal lattice parameters obtained by *ab initio* geometric optimization of the crystal structure [6, 7, 23]. For visual clarity, Fig. 4 shows the Curie temperatures as functions of the concentrations of *Me* = Al, Ga, Ge atoms along the experimental and theoretical dependences of the lat-

tice parameters estimated for all the alloys under consideration (Fig. 3). It can be seen that considering both the experimental and theoretical values of a_0 when calculating the T_C does not allow us to obtain a dependence corresponding to the experimental $T_C(x)$.

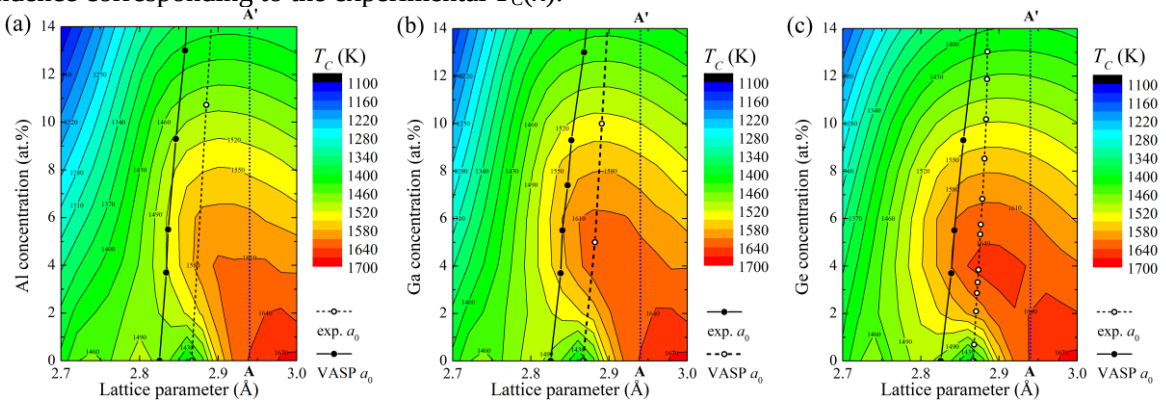

Fig. 3. Distribution of the Curie temperature for alloys: (a) $Fe_{100-x}Al_x$, (b) $Fe_{100-x}Ga_x$, and (c) $Fe_{100-x}Ge_x$, depending on the crystal lattice parameter *a* and the *Me* = Al, Ga, Ge concentration *x*. Solid (open) circles are experimental (obtained from geometric optimization using the VASP software package) dependences of the crystal lattice parameters; AA' is the distribution cross-section

The figure shows that maximum Curie temperature corresponds to the concentration range of $4 \le x \le 8$ at. %. The Curie temperature increases below this range and decreases above it. Nevertheless, such a cross-section (AA') can be found in these distributions (Fig. 3), along which the Curie temperature dependence changes from higher to lower with increasing concentration of the alloying element and is qualitatively in agreement with the experimental dependence. This cross-section can be constructed for the parameter $a \ge 2{,}94$ Å for all alloys. As can be seen from Fig. 4, for this value of the crystal lattice parameter, the Curie temperature decreases with increasing concentration of *Me* = Al, Ga, Ge.

The final thing to note from the analysis of the Curie temperature distribution is the absence of a direct correlation between the distribution of the largest interactions (between the nearest neighboring Fe atoms) and the distribution of the Curie temperature. From this, we conclude that the value of the Curie temperature is in a complex nonlinear dependence on the magnetic exchange interaction parameters.

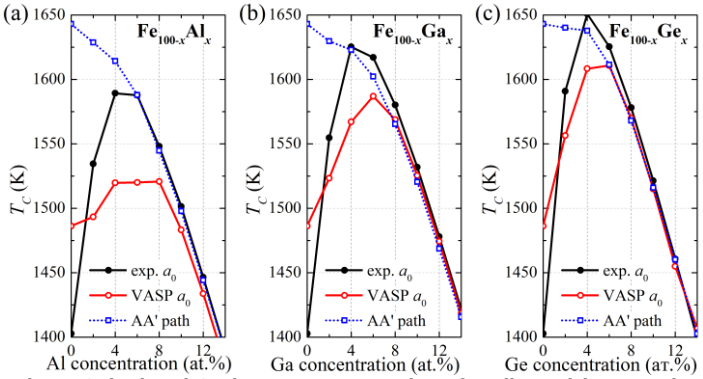

Fig. 4. Calculated Curie temperature values for alloys: (a) $Fe_{100-x}Al_x$, (b) $Fe_{100-x}Ga_x$, and (c) $Fe_{100-x}Ge_x$, obtained with experimental, theoretical (by *ab initio* geometric optimization) parameters of the crystal lattice, and along the cross-section AA' in Fig. 3 (*a* = 2,94 Å)

Conclusion

In this work, for $Fe_{100-x}Me_x$ alloys (*Me* = Al, Ga, Ge, $0 \le x \le 14$ at. %), the constants of magnetic exchange interaction J_{ij} are calculated within the density functional theory and the Curie temperatures T_C are estimated within the mean field approximation for the disordered phase *A2* in the crystal lattice parameter range of $2{,}7 \le a \le 3{,}0$ Å. The distribution of constants J_{ij} obtained in the work has a nonlinear behavior. The strongest interaction observed between the nearby Fe atoms is ferromagnetic and is ≈23 meV. In the second coordination sphere, the ferromagnetic interaction between Fe atoms is preserved and varies within 4–14 meV. In the third coordination sphere, antiferromagnetic exchange interaction is observed, which reaches a value of ≈ –2,5 meV. Estimation of the Curie temperature using the mean field approximation yields overestimated values compared to the experimental results. The Curie temperatures obtained with the experimental parameters of the crystal lattice have concentration dependences different from those observed experimentally, namely, they have a maximum Curie temperature in the concentration range of $4 \le x \le 8$ at. %. On the obtained distributions of the Curie temperature depending on the lattice constant and the content of *Me* = Al, Ga, Ge in $Fe_{100-x}Me_x$ alloys, it is possible to obtain concentration dependences that qualitatively describe the decreasing behavior of $T_C(x)$ ob-

served experimentally. The study shows that the Curie temperature value is in a complex nonlinear dependence on both the crystal structure constant and the parameters of the magnetic exchange interaction.

This study was supported by the Russian Science Foundation, project no. 24-22-20086, https://rscf.ru/project/24-22-20086/.

References

1. Golovin I.S., Palacheva V.V., Mohamed A.K., Balagurov A.M. Structure and Properties of Fe–Ga Alloys as Promising Materials for Electronics. *Physics of Metals and Metallography*, 2020, Vol. 121, pp. 851–893. DOI: 10.1134/S0031918X20090057.

2. Clark A.E., Hathaway K.B., Wun-Fogle M., Restorff J.B., Lograsso T.A., Keppens V.M., Petculescu G., Taylor R.A. Extraordinary Magnetoelasticity and Lattice Softening in BCC Fe-Ga Alloys. *Journal of Applied Physics*, 2003, Vol. 93, Iss. 10, pp. 8621–8623. DOI: 10.1063/1.1540130.

3. Balagurov A.M., Golovin I.S. Neutron Scattering in Studies of Fe-based Functional Alloys (Fe–Ga, Fe–Al). *Physics-Uspekhi*, 2021, Vol. 64, Iss. 7, pp. 702–721. DOI: 10.3367/UFNe.2020.11.038886.

4. Zagrebin M.A., Matyunina M.V., Sokolovskiy V.V., Buchelnikov V.D. The Effect of Exchange-Correlation Potentials on Magnetic Properties of Fe-(Ga, Ge, Al) Alloys. *Journal of Physics: Conference Series*, 2019, Vol. 1389, p. 012087. DOI: 10.1088/1742-6596/1389/1/012087.

5. Zagrebin M.A., Matyunina M.V., Koshkin A.B., Sokolovskiy V.V., Buchelnikov V.D. Structural and Magnetic Properties of Fe–Al alloys: Ab initio Studies. *Journal of Magnetism and Magnetic Materials*, 2022, Vol. 557, p. 169437. DOI: 10.1016/j.jmmm.2022.169437.

6. Zagrebin M.A., Matyunina M.V., Tarasova Yu.S., Sokolovskiy V.V., Buchelnikov V.D. The Effect of Structural Disorder on Magnetic Properties of Fe-Ga Alloys: Insights from Ab initio and Monte Carlo Calculations. *Journal of Superconductivity and Novel Magnetism*, 2025, Vol. 38, Article no. 136. DOI: 10.1007/s10948-025-06979-8.

7. Pavlukhina O.O., Matyunina M.V., Zagrebin M.A., Sokolovskiy V.V., Buchelnikov V.D., Zotov I.S. Magnetic Properties of Fe-(Ga,Ge) Compounds: Insights from Ab initio and Monte Carlo Simulations. *Journal of Superconductivity and Novel Magnetism*, 2025, Vol. 38, Article no. 157. DOI: 10.1007/s10948-025-07000-y.

8. Ebert H., Ködderitzsch D., Minár J. Calculating Condensed Matter Properties using the KKR-Green's Function Method – Recent Developments and Applications. *Reports on Progress in Physics*, 2011, Vol. 74, no. 9, p. 096501. DOI: 10.1088/0034-4885/74/9/096501.

9. Liechtenstein A.I., Katsnelson M.I., Antropov V.P., Gubanov V.A. Local Spin Density Functional Approach to the Theory of Exchange Interactions in Ferromagnetic Metals and Alloys. *Journal of Magnetism and Magnetic Materials*, 1987, Vol. 67, Iss. 1, pp. 65–74. DOI: 10.1016/0304-8853(87)90721-9.

10. Perdew J.P., Burke K., Ernzerhof M. Generalized Gradient Approximation Made Simple. *Physical Review B*, 1996, Vol. 77, p. 3865. DOI: 10.1103/PhysRevLett.77.3865.

11. Anderson P.W. Theory of Magnetic Exchange Interactions: Exchange in Insulators and Semiconductors. *Solid State Physics*, 1963, Vol. 14, pp. 99–214. DOI: 10.1016/S0081-1947(08)60260-X.

12. Borrego J.M., Blázquez J.S., Conde C.F., Conde A., Roth S. Structural Ordering and Magnetic Properties of Arc-Melted FeGa Alloys. *Intermetallics*, 2007, Vol. 15, Iss. 2, pp. 193–200. DOI:10.1016/j.intermet.2006.05.007.

13. Matyunina M., Zagrebin M., Sokolovskiy V., Buchelnikov V. Ab initio Study of Magnetic and Structural Properties of Fe-Ga Alloys. *EPJ Web of Conferences*, 2018, Vol. 185, pp. 04013. DOI: 10.1051/epjconf/201818504013.

14. Matyunina M.V.,Zagrebin M.A., Sokolovskiy V.V., Buchelnikov V.D. Magnetic properties of $Fe_{100-x}Ga_x$: Ab initio and Monte Carlo Study. *Journal of Magnetism and Magnetic Materials*, 2019, Vol. 470, pp. 118–122. DOI: 10.1016/j.jmmm.2017.11.011.

15. Zagrebin M.A., Matyunina M.V., Miroshkina O.N., Pavlukhina O.O., Sokolovskiy V.V., Buchelnikov V.D. Phase Transitions in Fe_3Al-based Alloys: Ab initio Study. *Phase Transitions*, 2020, Vol. 93, iss. 1, pp. 43–53. DOI: 10.1080/01411594.2019.1695255

16. Matyunina M.V., Zagrebin M.A., Sokolovskiy V.V., Buchelnikov V.D. First Principles Study of Structural and Magnetic Properties in $Fe_{100-x}Ge_x$ alloys. *Physica B: Condensed Matter*, 2020, Vol. 580, p. 411934. DOI: 10.1016/j.physb.2019.411934

17. Matyunina M.V., Zagrebin M.A., Buchelnikov V.D. Structural, Magnetic and Magnetocaloric Properties of Fe-Ga Alloys. *Chelyabinsk Physical and Mathematical Journal*, 2020, Vol. 5, Iss. 4(2), pp. 580–591. DOI: 10.47475/2500-0101-2020-15417.

18. Koshkin A.B., Zagrebin M.A., Sokolovskiy V.V., Buchelnikov V.D. First-Principles Studies of the Phase Transitions in Fe-Si Alloys. *Bulletin of the South Ural State University. Series of "Mathematics. Mechanics. Physics"*, 2021, Vol. 13, no. 1, pp. 52–58. DOI: 10.14529/mmph210106

19. Koshkin A.B., Zagrebin M.A., Matyunina M.V., Buchelnikov V.D. Structural and Magnetic phase Transitions in $Fe_{100-x}Al_x$ Alloys: an Ab inito Study. *Materials. Technologies. Design*, 2021, Vol. 3, no. 4(6), pp. 20–25. DOI: 10.54708/26587572_2021_34620.

20. Stein F., Palm M. Re-Determination of Transition Temperatures in the Fe-Al System by Differential Thermal Analysis. *International Journal of Materials Research*, 2007, Vol. 98, Iss. 7, pp. 580–588. DOI: 10.3139/146.101512.

21. Golovin I.S., Neuhäuser H., Sinning H.-R., Siemers C. Structure and Anelasticity of Ordered and Disordered Fe–Ge Alloys. *Intermetallics*, 2010, Vol. 18, Iss. 5, pp. 913–921. DOI: 10.1016/j.intermet.2009.12.031.

22. Kubaschewski O. *Iron-Binary Phase Diagrams*. Springer Berlin, Heidelberg, 1982, 185 p. DOI: 10.1007/978-3-662-08024-5

23. Tarasova Yu.S., Matyunina M.V. Vliyanie atomnogo besporyadka na magnitnye svoystva kristallicheskoy reshetki A2 splavov Fe-Z (Z = Ga, Ge, Al) (Influence of Atomic Disorder on the Magnetic Properties of the A2 Crystal Lattice of Fe-Z (Z = Ga, Ge, Al) alloys). *Yuzhno-Ural'skaya molodezhnaya shkola po matematicheskomu modelirovaniyu: sbornik trudov VII Vserossiyskoy nauchno-prakticheskoy konferentsii 14–15 iyunya 2024 g.* (South Ural Youth School on Mathematical Modeling: Collection of Papers of the VII All-Russian Scientific and Practical Conference June 14–15, 2024). Chelyabinsk: Publishing center of SUSU, 2024, pp. 65–69. (in Russ.).

Received June 3, 2025

Information about the authors

Zagrebin Mikhail Aleksandrovich is Dr. Sc. (Physics and Mathematics), Associate Professor, Professor, Radiophysics and Electronics Department, Chelyabinsk State University, Chelyabinsk, Russian Federation, e-mail: miczag@mail.ru.

Markovich Ivan Alekseevich is Post-graduate Student, Mathematical and Computer Modeling Department, South Ural State University, Chelyabinsk, Russian Federation.

Kuznetsov Andrey Sergeevich is Laboratory Assistant, Researcher, Condensed Matter Physics Department, Chelyabinsk State University, Chelyabinsk, Russian Federation.

Matyunina Mariya Viktorovna, is Cand. Sc. (Physics and Mathematics), Associate Professor, Condensed Matter Physics Department, Chelyabinsk State University, Chelyabinsk, Russian Federation, e-mail: matunins.fam@mail.ru.

Butakov Anatoliy Vladimirovich is Cand. Sc. (Physics and Mathematics), Associate Professor, Radiophysics and Electronics Department, Chelyabinsk State University, Chelyabinsk, Russian Federation.

Bulletin of the South Ural State University
Series "Mathematics. Mechanics. Physics"
2025, vol. 17, no. 3, pp. 47–54

УДК 537.61 **DOI: 10.14529/mmph250305**

КОМПЬЮТЕРНОЕ МОДЕЛИРОВАНИЕ МАГНИТНЫХ СВОЙСТВ НЕУПОРЯДОЧЕННОЙ ОЦК ФАЗЫ СПЛАВОВ $Fe_{100-X}Me_X$ (*Me* = AL, GA, GE)

М.А. Загребин[1], И.А. Маркович[2], А.С. Кузнецов[1], М.В. Матюнина[1], А.В. Бутаков[1]
[1] Челябинский государственный университет, г. Челябинск, Российская Федерация
[2] Южно-Уральский государственный университет, г. Челябинск, Российская Федерация
E-mail: miczag@mail.ru

Аннотация. Для сплавов Fe-*Me* (*Me* = Al, Ga, Ge) в рамках теории функционала плотности рассчитаны постоянные магнитного обменного взаимодействия J_{ij} и проведена оценка темпера-

туры Кюри T_C для неупорядоченной фазы *A*2 в интервале концентраций *Me* = Al, Ga, Ge $0 \le x \le 14$ ат. % и диапазоне параметров кристаллической решетки $2{,}7 \le a \le 3{,}0$ Å. Полученное в работе распределение J_{ij} демонстрирует нелинейное поведение. Наибольшее ферромагнитное взаимодействие в первой координационной сфере составляет ≈ 23 мэВ. В третьей координационной сфере наблюдается антиферромагнитное обменное взаимодействие, которое достигает значения ≈ –2,5 мэВ. Температуры магнитного перехода, рассчитанные с использованием приближения молекулярного поля на основании экспериментальных значений и параметров a_0, рассчитанных в рамках теории функционала плотности, показывают наличие концентрационного интервала $4 \le x \le 8$ ат. %, в котором T_C возрастает. Сечение распределения рассчитанных значений температуры Кюри показывает, что для всех исследуемых сплавов Fe-*Me* (*Me* = Al, Ga, Ge) при параметре решетки a_0 = 2,94 Å возможно построить зависимость $T_C(x)$, удовлетворяющую экспериментальной.

Ключевые слова: сплавы на основе Fe; первопринципные расчеты; магнитное обменное взаимодействие, температура Кюри.

Литература

1. Структура и свойства Fe–Ga-сплавов – перспективных материалов для электроники / И.С. Головин, В.В. Палачева, А.К. Мохамед, А.М. Балагуров // Физика металлов и металловедение. – 2020. – Т. 121, № 9. – С. 937–980.

2. Extraordinary Magnetoelasticity and Lattice Softening in BCC Fe-Ga Alloys / A.E. Clark, K.B. Hathaway, M. Wun-Fogle *et al.* // J. of Applied Physics. – 2003. – Vol. 93, Iss. 10. – P. 8621–8623.

3. Балагуров, А.М. Рассеяние нейтронов в исследованиях функциональных сплавов на основе железа (Fe–Ga, Fe–Al) / А.М. Балагуров, И.С. Головин // УФН. – 2021. – Т. 191, № 7. – С. 738–759.

4. The Effect of Exchange-Correlation Potentials on Magnetic Properties of Fe-(Ga, Ge, Al) alloys / M.A. Zagrebin, M.V. Matyunina, V.V. Sokolovskiy, V.D. Buchelnikov // Journal of Physics: Conference Series. – 2019. – Vol. 1389. – P. 012087.

5. Structural and Magnetic Properties of Fe–Al Alloys: *Ab initio* Studies / M.A. Zagrebin, M.V. Matyunina, A.B. Koshkin *et al.* // J. of Magnetism and Magnetic Materials. – 2022. – Vol. 557. – P. 169437.

6. The Effect of Structural Disorder on Magnetic Properties of Fe-Ga Alloys: Insights from Ab initio and Monte Carlo Calculations / M.A. Zagrebin, M.V. Matyunina, Yu.S. Tarasova *et al.* // J. of Superconductivity and Novel Magnetism. – 2025. – Vol. 38. – Article no. 136.

7. Magnetic Properties of Fe-(Ga,Ge) Compounds: Insights from Ab initio and Monte Carlo Simulations / O.O. Pavlukhina, M.V. Matyunina, M.A. Zagrebin *et al.* // J. of Superconductivity and Novel Magnetism. – 2025. – Vol. 38. – Article no. 157.

8. Ebert, H. Calculating Condensed Matter Properties using the KKR-Green's Function Method – Recent Developments and Applications / H. Ebert, D. Ködderitzsch, J. Minár // Reports on Progress in Physics. – 2011. – Vol. 74, no. 9. – P. 096501.

9. Local Spin Density Functional Approach to the Theory of Exchange Interactions in Ferromagnetic Metals and Alloys / A.I. Liechtenstein, M.I. Katsnelson, V.P. Antropov, V.A. Gubanov // Journal of Magnetism and Magnetic Materials. – 1987. – Vol. 67, Iss. 1. – P. 65–74.

10. Perdew, J.P. Generalized Gradient Approximation Made Simple / J.P. Perdew, K. Burke, M. Ernzerhof // Physical Review B. – 1996. – Vol. 77. – P. 3865. [Erratum Phys. Rev. Lett. 78, 1396 (1997)]

11. Anderson, P.W. Theory of Magnetic Exchange Interactions: Exchange in Insulators and Semiconductors / P.W. Anderson // Solid State Physics. – 1963. – Vol. 14. – P. 99–214.

12. Structural Ordering and Magnetic Properties of Arc-Melted FeGa Alloys / J.M. Borrego, J.S. Blázquez, C.F. Conde *et al.* // Intermetallics. – 2007. – V. 15, Iss. 2. – P. 193–200.

13. Ab initio Study of Magnetic and Structural Properties of Fe-Ga Alloys / M. Matyunina, M. Zagrebin, V. Sokolovskiy, V. Buchelnikov // EPJ Web of Conferences. – 2018. – Vol. 185. – P. 04013.

14. Magnetic Properties of $Fe_{100-x}Ga_x$: Ab initio and Monte Carlo Study / M.V. Matyunina, M.A. Zagrebin, V.V. Sokolovskiy, V.D. Buchelnikov // J. of Magnetism and Magnetic Materials. – 2019. – Vol. 470. – P. 118–122.

15. Phase Transitions in Fe_3Al-Based Alloys: Ab initio Study / M.A. Zagrebin, M.V. Matyunina, O.N. Miroshkina *et al.* // Phase Transitions. – 2020. – Vol. 93, Iss. 1. – P. 43–53.

16. Matyunina, M.V. First Principles Study of Structural and Magnetic Properties in $Fe_{100-x}Ge_x$ Alloys / M.V. Matyunina, M.A. Zagrebin, V.V. Sokolovskiy, V.D. Buchelnikov // Physica B: Condensed Matter. – 2020. – Vol. 580. – P. 411934.

17. Структурные, магнитные и магнитокалорические свойства сплавов Fe-Ga / М.В. Матюнина, В.В. Соколовский, М.А. Загребин, В.Д. Бучельников // Челябинский физико-математический журнал. – 2020. – Т. 5, no. 4-2. – С. 580–591.

18. First-Principles Studies of the Phase Transitions in Fe-Si Alloys / А.Б. Кошкин, М.А. Загребин, В.В. Соколовский, В.Д. Бучельников // Вестник ЮУрГУ. Серия «Математика. Механика. Физика». – 2021. – Т. 13, № 1. – С. 52–58.

19. Структурные и магнитные фазовые превращения в сплавах $Fe_{100-x}Al_x$: исследования ab inito / А.Б. Кошкин, М.А. Загребин, М.В. Матюнина, В.Д. Бучельников // Materials. Technologies. Design. – 2021. – Т. 3, № 4(6). – С. 20–25.

20. Stein, F. Re-Determination of Transition Temperatures in the Fe-Al System by Differential thermal Analysis / F. Stein, M. Palm // International Journal of Materials Research. – 2007. – Vol. 98, Iss. 7. – P. 580–588.

21. Structure and Anelasticity of Ordered and Disordered Fe–Ge Alloys / I.S. Golovin, H. Neuhäuser, H.-R. Sinning, C. Siemers // Intermetallics. – 2010. – Vol. 18, Iss. 5. – P. 913–921.

22. Kubaschewski, O. Iron-Binary Phase Diagrams / O. Kubaschewski. – Berlin, Springer, 1982. – 185 p.

23. Тарасова, Ю.С. Влияние атомного беспорядка на магнитные свойства кристаллической решетки A2 сплавов Fe-Z (Z = Ga, Ge, Al) / Ю.С. Тарасова, М.В. Матюнина // Южно-Уральская молодежная школа по математическому моделированию: сборник трудов VII Всероссийской научно-практической конференции 14–15 июня 2024 г. – Челябинск: Издательский центр ЮУрГУ, 2024. – С. 65–69.

Поступила в редакцию 3 июня 2025 г.

Сведения об авторах

Загребин Михаил Александрович – доктор физико-математических наук, доцент, профессор кафедры радиофизики и электроники, Челябинский государственный университет, г. Челябинск, Российская Федерация, e-mail:miczag@mail.ru.

Маркович Иван Алексеевич – аспирант, кафедра «Математическое и компьютерное моделирование», Южно-Уральский государственный университет (национальный исследовательский университет), г. Челябинск, Российская Федерация.

Кузнецов Андрей Сергеевич – лаборант-исследователь кафедры физики конденсированного состояния, Челябинский государственный университет, г. Челябинск, Российская Федерация.

Матюнина Мария Викторовна – кандидат физико-математических наук, доцент кафедры физики конденсированного состояния, Челябинский государственный университет, г. Челябинск, Российская Федерация, e-mail: matunins.fam@mail.ru.

Бутаков Анатолий Владимирович – кандидат физико-математических наук, доцент кафедры радиофизики и электроники, Челябинский государственный университет, г. Челябинск, Российская Федерация.