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Electronic structure modification and negative magnetostriction in Fe-Ga alloy of $D0_3$ structure with Ga content variation

Abstract. The influence of a change in the Ga content on the magnetostrictive properties of the Fe3Ga alloy with the D03 structure has been studied by density functional theory methods. The change in the stoichiometry of the alloy under study was carried out by replacing the Fe atoms with Ga. The replacement leads to a significant change in the electronic structure of the systems under study, which leads to a significant increase in the density of electronic states near the Fermi level. This effect leads to an increase in the magnetoelastic energy, which leads to an increase in the value of the magnetostrictive coefficient $\lambda 001$. A further increase in $\lambda 001$ occurs due to a decrease in the shear modulus, which occurs due to an increase in the number of loosening bonds in the system with an increase in the Ga content. The resulting dependence of $\lambda 001$ on the Ga content, although they show an increase in the absolute value of the coefficient $\lambda 001$, but give its negative values, in contrast to the positive value of magnetostriction observed in the experiment. Solving the problem of matching the sign of the theoretical and experimental values of the magnetostrictive coefficients requires further research.
Keywords: Fe-Ga alloy, electronic structure, density functional theory, magnetostriction, magnetoelastic energy.

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1. Introduction

Materials with high magnetostriction are widely used as magnetic field sensors, magneto-mechanical actuators, and energy collectors [1]. A significant magnetic field characteristic is needed [2]. Giant magnetostriction up to 2000 ppm was found in rare-earth iron-based alloys Terfenol and Terfenol-D [3,4]. However, the cost of these materials is high due to the use of rare earth elements. In addition, their hardness and brittleness are very high, limiting the materials' scope.

Binary $Fe_{1-x}Ga_x$ alloys (Galfenol), although having inferior magnetostrictive properties to Terfenol-D, are attractive due to their low cost and high mechanical strength, low saturation magnetic field, excellent ductility, and low cost [5-7]. $Fe_{1-x}Ga_x$ alloys demonstrate the two-peak tetragonal magnetostrictive coefficient λ_{001} behavior near x = 0.19 and x=0.27 with the value of the magnetostrictive coefficient as large as 400 ppm [8-10]. It was found experimentally that the peak magnetostriction values at 19% Ga is associated with maximum value of the magnetoelastic coupling constant as a function of the Ga concentration. The second magnetostriction peak can be attributed to softening of the elastic modules $c^J = (c_{11} - c_{12})/2$ [6].

According to the phase diagram proposed by Koster at al. [11] and Kubashevski [12] and supported by Golovin et. al. [13] the equilibrium structure of Fe-26.9Ga and Fe-25.5 Ga alloys at room temperature (RT) must be 100% $L1_2$ phase and about 90%$L1_2$ + 10%A2 phase respectively. Using high resolution neutron diffraction, it was proven that the initial state of FeGa functional alloys with 25 and 27 at. % Ga as-cast samples at room temperature is the $D0_3$ phase which results from ordering of the high temperature A2 phase during cooling. From the analysis of the diffraction peak widths, it was concluded that the initial state consists of domains of about 1400-1800 *Å* in size with long-range ordered $D0_3$ with lattice

parameters 5.8130 – 5.8172 $\dot{A}$ [14]. Upon heating, there is an irreversible first-order phase transition from the metastable $D0_3$ to the equilibrium L_21 phase [13,15,16]. A2 and $D0_3$ – structured $Fe_{1-x}Ga_x$ alloys have positive magnetostriction, but the L_21-structured one has negative magnetostriction [13,14,17,18].

Studies of the magnetostriction and elastic properties of the Fe-Ga alloys with a Ga content of about 25 at. % showed that a small, within 25 at. %, change in the Ga content sharply affects the value of the magnetostriction coefficient and the elastic modulus c' [6,19,20]. If for the Fe-Ga alloy of structure $D0_3$ the measured value of the magnetosrictive coefficient 3/2 λ_{001} is 150 ppm (λ_{001} = 100) [14], then for the Fe-27.2Ga this value reaches 350 ppm [6,19]. According to the results of the theoretical modeling, the value 3/2 λ_{001} is negative and equals -161 ppm ($\lambda_{001} = -107\ ppm$) [21].

In this work, we study the effect of changing the gallium content in the Fe_3Ga alloy with the $D0_3$ structure on the magnetostriction coefficients λ_{001}. Calculations have shown that, at small changes in the composition of the compound under study near the Fermi level, there is a sharp increase in the number of d-states of Fe atoms, which leads to an increase in the magnetoelastic energy. Also an increase in the Ga content leads to an increase in the number of antibonding states, as a result of which the value of the shear rmodulus of elasticity c' decreases. Both effects leads to an increase in absolute value of λ_{001}. However, the difference in the sign of the calculated an experimental values of the magnetostriction coefficients remains unclear.

2. Computation Details

The $D0_3$ ($Fm\bar{3}m$, group 225) unit cell consist of three Fe and one Ga site (Fig. (1(a)). There are two types of Fe atoms: those with Fe and Ga atoms in nearest-neighboring positions (Fe1) and those with only Fe atoms in the nearest-neighboring positions (Fe2). The ocal order around the Fe1 and Fe 2 atoms is shown in Figs. 1 (b,c), correspondingly. A 2x2x2 cubic supercell (128 atoms/cell) was used to model small chemical composition changes on the physical properties of compound under investigation.

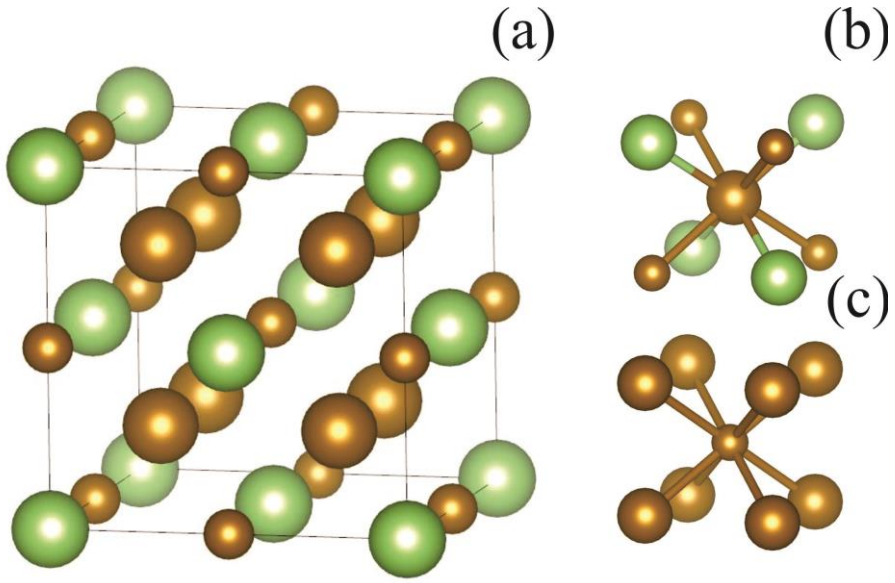

Figure 1. (a) Unit cell of the Fe_3Ga alloy with the $D0_3$ structure. Local environment of atoms of type (b) Fe1 and (c) Fe2. Golden and green balls represent Fe and Ga atoms, respectively. Large balls denote Fe1 atoms, and small balls –Fe2

The coefficient of tetragonal magnetostriction at volume-constant distortion ($\varepsilon_x = \varepsilon_y = -1/2\varepsilon_z$) Depends on the ratio of magnetoelastic energy b_1 and tetragonal shear modulus c' and is written as

$$\lambda_{001} = -\frac{b1}{3c'} \quad (1)$$

where $b_1 = -\frac{2}{3V_0}\frac{dE_{MCA}}{d\varepsilon_z}$ is determined by the dependence of the magnetocrystalline anisotropy energy E_{MCA} on distortion [22,23]. The elastic constants c_{11} and c_{12} were obtained by the stress-strain relation $\sigma_i = c_{ij}\varepsilon_j$.

From the electronic structure, the enhancement of the magnetostrictive effect in Fe-Ga alloy is a high dependence of magnetocrystalline anisotropy energy (E_{MCA}) on the strain. The appereance of nonbinding d-states of electrons of Fe atoms near the Fermi level is accompanied by an increase in electronic density of states (DOS) of the Fe atoms closest to Ga, particularly from states in the minority spin channel. This effect ensures the growth of E_{MCA} on the one hand and a decrease in elastic moduli, on the other hand, increasing the overall magnetostrictive effect [24,25].

We recall that the spin-orbit coupling (SOC) is the key factor for E_{MCA}. The lowest order contribution of SOC toward the total energy is [26]

$$E^{SOC} = -\zeta^2 \sum_{o,u} \frac{[\langle o|\hat{\sigma}\cdot\hat{L}|u\rangle]^2}{\varepsilon_u - \varepsilon_o}, \quad (2)$$

where $|o\rangle >$ and $|u\rangle >$ represent the sets of occupied and unoccupied states, respectively. The nonzero contributions from the d -states to E^{SOC} are from the following matrix elements

$$\langle xy|\hat{\hat{L}}_z|yz\rangle = 1, \langle x^2 - y^2|\hat{\hat{L}}_z xz\rangle = 2, \langle z^2|\hat{\hat{L}}_x xz, yz\rangle = \sqrt{3},$$
$$\langle xy\left|\hat{\hat{L}}_x\right| xz, yz\rangle = 1, \langle x^2 - y^2|\hat{\hat{L}}_z xz, yz\rangle = 1$$

The first-principles calculations of structural and magnetic properties of the Fe-Ga alloy systems were done by means of the VASP (Vienna Ab-initio Simulation Package) [27, 28] with the supercell approach. The exchange-correlation potential was treated by the generalized gradient approximation (GGA) in Perdew-Burke-Ernzerhof (PBE) form [29]. The k-point mesh was generated by the Monkhorst-Pack scheme [23] with a grid of 4x4x4 points. To describe electron-ion interactions, the PAW pseudopotentials [20, 21] were applied and the valence-electron configuration of Fe($3s^2 3p^6 3d^7 4s^1$) and Ga ($3d^{10} 4s^2 4p^1$) were selected. The value of the the plane-wave cut-off energy is 500 eV. Lattice parameters were relaxed to zero pressure while retaining the cubic symmetry. To obtain the ground structure, internal structure parameters were optimized until the remaining forces were less than 0.01 eV/$\dot{A}$. All calculations were done at T =0 K.

Structures were visualized in the VESTA package [30]. We used the VASPKIT code for post-processing of the VASP calculated data [31].

3. Results and Discussion

The study of changing the chemical composition of the Fe_3Ga alloy of structure $D0_3$ towards an increase in the Ga content was carried out by replacing Fe atoms with Ga atoms. Calculations have shown that, with such a substitution, it is more energetically favorable to place an additional Ga atom at the Fe2 site than at the Fe1 site. The difference in the energies of the model supercells is 0.121 eV. This finding is consistent with the fact that gallium atoms in Fe-Ga alloys are not located at the nearest lattice sites, and the probability of finding gallium atoms at neighboring sites is negligible [22]. Further modeling of the properties of the compound under study was carried out for cases where Ga replaced the Fe2 atoms. We studied structures in which up to 3 Fe atoms were replaced, corresponding to the maximum Ga content of 27.35 at.%. The substitution was carried out so that the distances between the replaced atoms were maximum. As a result, the interatomic distances are no less than 7$\dot{A}$. In what follows, we consider configurations in which atoms of the Fe2 type are substituted unless otherwise noted.

The results of calculations of the magnetostriction coefficient λ_{001} in comparison with the experimental results are presented in Fig. 2. The obtained theoretical data are in good agreement with the measurement results and show a sharp increase in the value of λ_{001} with a slight change in the Ga content.

According to Eq. 1, an increase in λ_{001} is possible in the case of an increase in the magnetoelastic energy b_1 or a decrease in the value of the elastic modulus c'. Changes in both of these quantities as a function of the content of Ga atoms are shown in Fig. 3 comparing with available literature data [6, 19, 20, 32-34]. When one Fe2 atom is replaced in the perfect $D0_3$ structure, the magnetoelastic energy increases by factor two, which further decreases linearly with an increase in the Ga content (Fig.3 (a)). The theoretical data obtained predict the possibility of a second peak in the value of the magnetoelastic energy at a Ga content close to 25 at.%. In the experiment [6], one peak in - b_1 value was observed near 19 at.%Ga. However, it should be noted that this peak lies in a relatively narrow region of Ga concentration, which makes it difficult to detect it. In addition, and much more importantly, the calculated sign of b1 is opposite to that measured experimentally but agrees with earlier calculations [21]. This difference is due to the sign of the derivative in Eq. 1.

The dependence of the elastic modulus c' on the Ga content is shown in Fig. 3 (b). When one Fe2 atom is replaced, the value of c' changes slightly. With a further change in the Ga content, this elastic modulus begins to decrease sharply, and at 27.35 at.% Ga, the structure becomes mechanically unstable due to the c' modulus turns to zero. In this case, to confirm the observed tendencies of c' change, we also performed additional calculations in which the Fe atom replaced the Ga atom, and Ga replaced four Fe2 atoms.

At a Ga content of 24-26 at.%, the calculated values of c' are in good agreement with the experimental data. As the Ga content increases, the discrepancy between theory and experiment becomes significant since the experiment did not reveal a decrease in the value of c' with a further increase in the Ga content. Stabilization of the $D0_3$ structure can occur by randomizing a small number of Ga atoms from their ordered lattice sites [25].

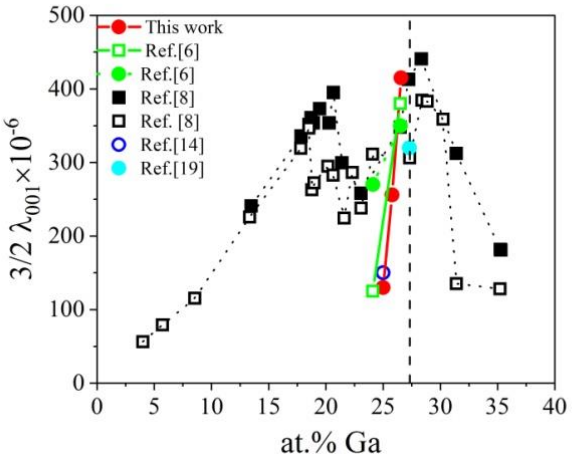

Figure 2. Calculated values of magnetostrictive coefficient λ_{001} along with the experimental data. It should be noted that the signs of the experimental and theoretically calculated values are different and here are the absolute values for the theoretically calculated values of λ_{001}. The dotted vertical line corresponds to the mechanical stability boundary of the $D0_3$ structure

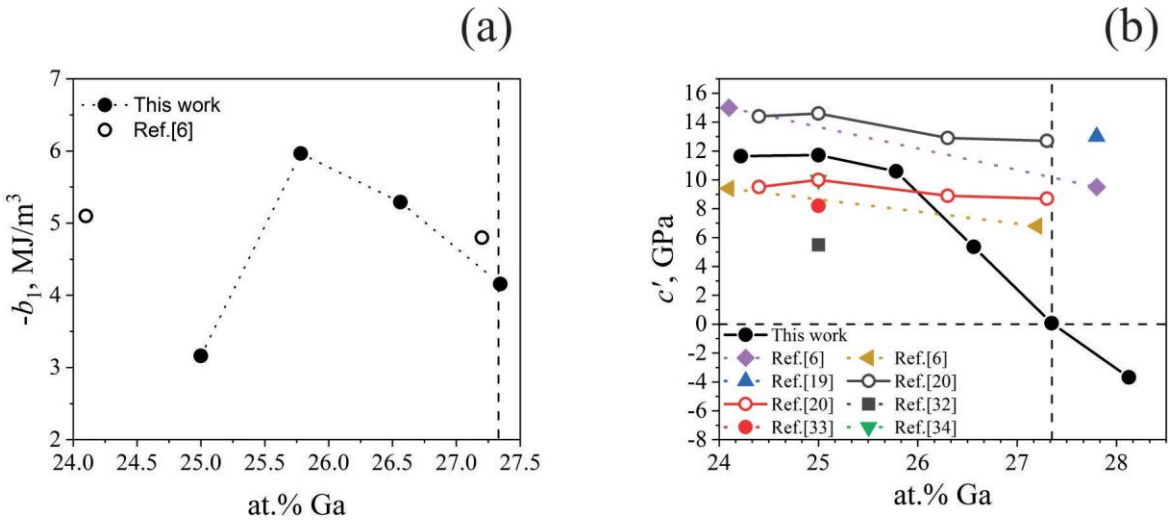

Figure 3. Calculated Ga-content dependent values of (a) magnetoelastic energy (with opposite sign) and (b) elastic modulus c′ along with experimental data. The dotted vertical line corresponds to the mechanical stability boundary of the $D0_3$ structure

When Ga replaces one Fe2 atom, the increase in the value of λ_{001} occurs due to the rise in the value of the magnetoelastic energy - b_1. Further growth of λ_{001} occurs because the elastic modulus c' decreases. To study why the value of - b_1 increases, we compared the density of electronic states of a perfect lattice $D0_3$ and structures in which one Ga atom substitutes the Fe atom. The results obtained are shown in Figs. 4 (a,b). A comparison of projected DOS (PDOS) for d -states on Fe atoms of the perfect structure $D0_3$ and a cell with one substituted Fe atom shows that even such a slight variation in the composition of the alloy leads to significant changes in the electronic structure. The changes are extreme for spin-up states for both types of atoms - Fe1 and Fe2. PDOS for spin-down d -states on atoms of the Fe2 type almost does not change with a variation in the composition of the alloy.

The resulting changes in the electronic structure have a critical effect on the magnetic anisotropy energy. As follows from Eq. 2, the SOC depends on the matrix elements calculated between the states near the Fermi level. Thus, an increase in the density of d -states on Fe atoms leads to an increase in the magnetic anisotropy energy, which in turn leads to a rise in the value of λ_{001}.

It should be noted that the change in PDOS on Fe atoms has a nonlocal character. PDOS of d -states on atoms of the Fe2 type upon substitution of Fe1 (Fig. 4 (c)) and Fe2 (Fig. 4 (d)) with Ga atoms undergo significant changes independent of the distance from the substituted Fe atom. This effect is very different from the changes in PDOS with a modification in the chemical composition of a disordered FeGa alloy of the A2 structure. The changes concern only the Fe atoms of the impurity atom's first and second coordination shells [35]. Such a nonlocal nature of the effect on the electronic structure in the $D0_3$ lattice is due to long-range order. A change in the composition leads to delocalized electronic states on Fe atoms. In disordered alloys, such states are localized near the impurity atom.

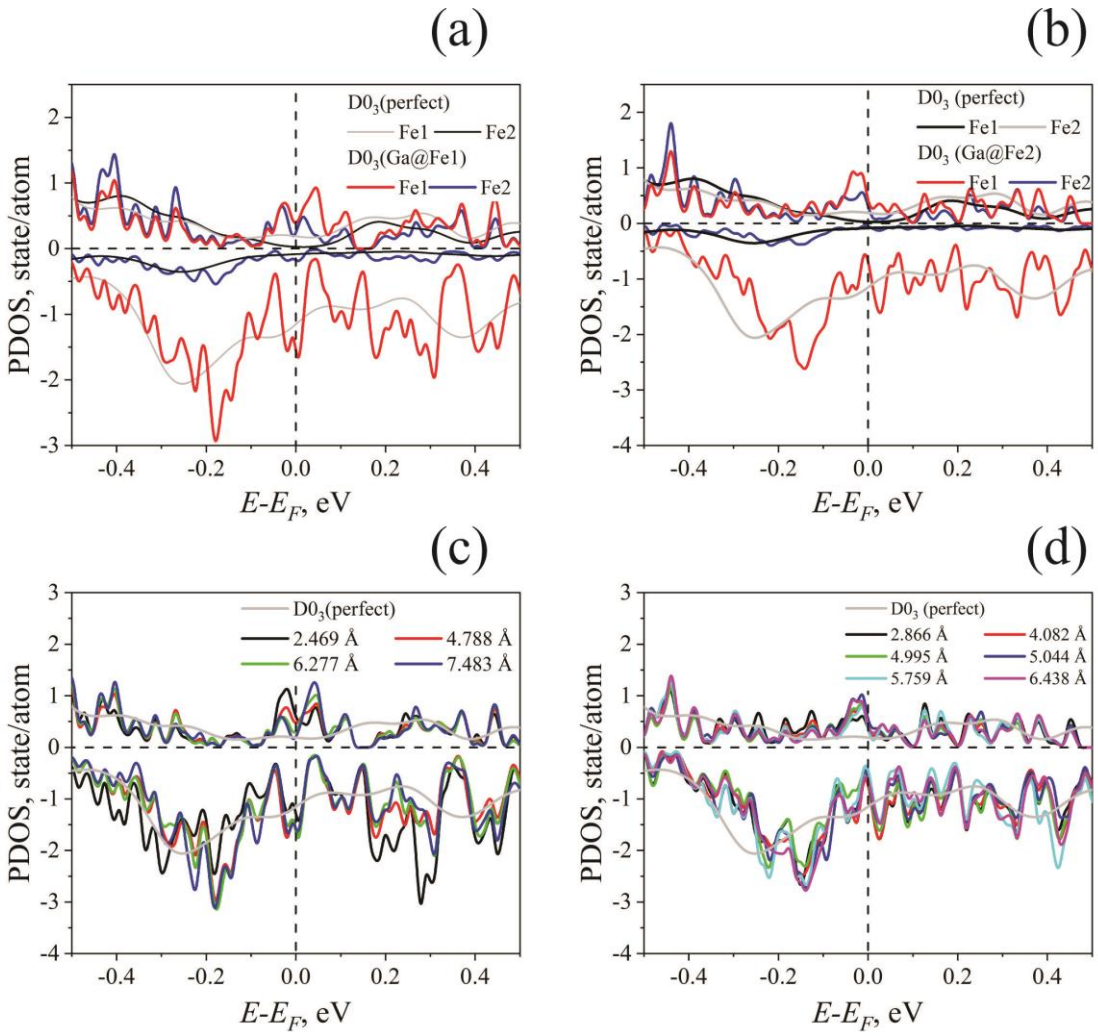

Figure 4. The projected density of states of d -electrons on Fe atoms when Ga replaces atoms of type (a) Fe1 and (b) Fe2 compared to the corresponding values for the perfect $D0_3$ structure. The distribution of densities of d -states on Fe1 atoms as a function of the distance from the Ga atom substituting for (c) Fe1 and (c) Fe2 atoms. Colored lines correspond to PDOS on Fe1 atoms at the indicated distances from the Ga atom substituting Fe

The fundamental difference lies in the fact that the density of antibonding d -states on atoms of the Fe1 type is much higher than on atoms of the Fe2 type [24, 25]. Ga content caused electronic structure modifications affecting spin-down electronic states contributed to changes in magnetostriction [22]. A quantitative description in Fig. 5 shows the number of electron states with spin down near the Fermi level of ± 0.2 eV, N(↓) on Fe atoms depending on the content of Ga atoms in the alloy. When one Fe2 atom is replaced, the value of N(↓) takes on a maximum value, which explains the peak in the value of the magnetoelastic energy shown in Fig. 3 (a). As the Ga content increases, the number of antibonding bonds in the system increases, which leads to a decrease in the elastic modulus c′, which corresponds to the instability of the crystal concerning shear distortions. (Fig. 3(b)). We attribute the decrease in the value of N(↓) to the violation of the coherence of electronic states due to Ga atoms replacing Fe atoms due to their random arrangement in the lattice. The value of N(↓), when replacing more than one Fe atom with a Ga atom and when replacing a Ga atom with Fe, takes values close to the maximum for the disordered Fe-20Ga alloy [22]. At the same time, this kind of disorder does not lead to any significant changes in the qualitative form of the PDOS graphs as it is seen in Fig. 6.

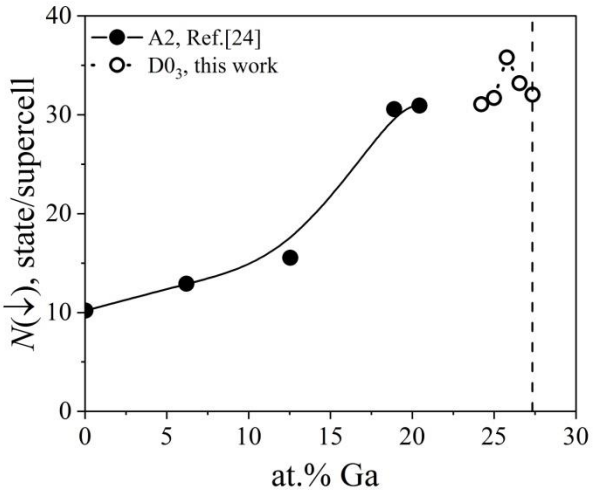

Figure 5. Calculated Ga-content dependent number of electronic states at the Fermi level in the minority spin channel, N(↓). The dotted vertical line corresponds to the mechanical stability boundary of the D0₃ structure

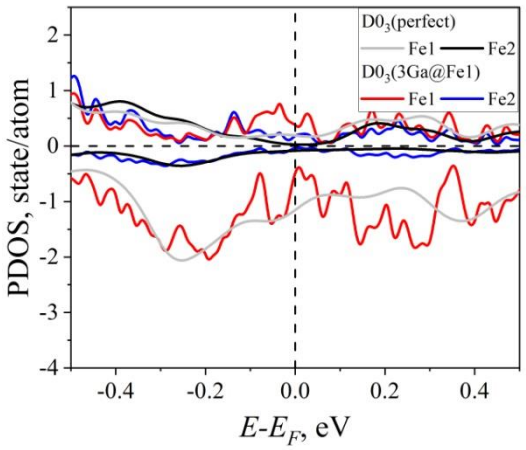

Figure 6. The density of states of d-electrons on Fe atoms for mechanically unstable Fe-27.35at.%Ga (three Ga replace atoms of Fe2 type) compared to the corresponding values for the perfect D0₃ structure

4. Conclusion

In this work, we study the effect of changing the stoichiometry of the D0₃ Fe₃Ga alloy on the electronic and elastic properties. The data obtained make allow to analyze the effect on the magnetostrictive properties of the considered compounds. Calculations showed that replacing a Fe atom with a Ga atom in the supercell of the D0₃ lattice leads to a significant change in the compound's electronic structure. As a result, the density of electronic d -states near the Fermi level increases, which leads to a rise in the magnetocrystalline energy. This effect leads to an increase in the magnitude of the magnetoelastic energy, but the value of the elastic modulus c' does not change, which leads to an increase in the magnetostrictive coefficient λ_{001} . The further increase in λ_{001} with increasing Ga content is due to a decrease in the elastic modulus c' with a slight reduction in the value of the magnetoelastic energy. The data obtained agree with the known experimental results. The data obtained agree with the known experimental results in absolute value but differ in the sign of the obtained values. We are currently searching for the reasons for this difference.

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References

1. A.E. Clark, K.B. Hathaway // Academic, San Diego. - 2000. - Ch. 1. - P. 1-48.
2. E. du Tremolet de Lacheisserie // Springer-Verlag, New York. - 2005. - P. 213-234.
3. F. Jerems, C.M. Mahon, A.G. Jenner, R.D. Greenough, Amorphous magnetic materials for transducers // Ferroelectrics. - 1999. - 228. -1. - P. 333-341. doi:https://doi.org/10.1080/00150199908226146.
4. J.D. Verhoeven, J.E. Ostenson, E.D. Gibson, O.D. McMasters, The effect of composition and magnetic heat treatment on the magnetostriction of TbxDy1xFey twinned single crystals // Journal of Applied Physics. -1989. - 66. - 2. -P. 772 - 779. doi:https://doi.org/10.1063/1.343496.
5. J. Atulasimha, A. B. Flatau, A review of magnetostrictive iron-gallium alloys // Smart Materials and Structures. -2011. - 20. - 4. - 043001. doi:10.1088/0964-1726/20/4/043001.
6. A.E. Clark, K.B. Hathaway, M. Wun-Fogle, J.B. Restorff, T.A. Lograsso, V.M. Keppens, G. Petculescu, R.A.Taylor, Extraordinary magnetoelasticity and lattice softening in bcc Fe-Ga alloys // Journal of Applied Physics. - 2003. - 93. - 10. - P. 8621-8623. doi:10.1063/1.1540130.
7. A.E. Clark, J.B. Restorff, M. Wun-Fogle, T.A. Lograsso, D. L. Schlagel, Magnetostrictive properties of body- centered cubic fe-ga and fe-ga-al alloys // IEEE Transactions on Magnetics. - 2000. - 36. - 5. - P. 3238-3240. doi:10.1109/20.908752.
8. Summers E.M., Lograsso T.A., Wun-Fogle M., Magnetostriction of binary and ternary Fe-Ga alloys // Journal of Materials Science. - 2007. - 42. -23. - P. 9582-9594. doi:https://doi.org/10.1007/s10853-007-2096-6.
9. Q. Xing, Y. Du, R. McQueeney, T. Lograsso, Structural investigations of fe-ga alloys: Phase relations and magnetostrictive behavior // Acta Materialia. - 2008. - 56. - 16. -P. 4536-4546. doi:https://doi.org/10.1016/j.actamat.2008.05.011.
10. A. Clark, M. Wun-Fogle, J. Restorff, K. Dennis, T. Lograsso, R. McCallum, Temperature dependence of the magnetic anisotropy and magnetostriction of Fe100?xGax (x=8.6, 16.6, 28.5) // Journal of Applied Physics. - 2005.- 97. - 10. 49th Annual Conference on Magnetism and Magnetic Materials, Jacksonville, FL, NOV 07-11, 2004 (MAY 15 2005). doi:10.1063/1.1856731.
11. W. Koster, T. Godecke, Uber den aufbau des systems eisen-gallium zwischen 10 und 50 at.-abhangigkeit von der warmebehandlung // International Journal of Materials Research. - 1977. - 68. - 10. - P. 661-666. doi:doi:10.1515/ijmr-1977-681003
12. O. Kubaschewski, Iron-Binary phase diagrams // Springer Science & Business Media. - 2013.
13. I. Golovin, A. Balagurov, V. Palacheva, A. Emdadi, I. Bobrikov, V. Cheverikin, A. Prosviryakov, S. Jalilzadeh, From metastable to stable structure: the way to construct functionality in Fe-27Ga alloy // Journal of Alloys and Compounds. - 2018. - 751. - P. 364-369. doi:10.1016/j.jallcom.2018.04.127.
14. I.S. Golovin, A.K. Mohamed, V.V. Palacheva, V.V. Cheverikin, A. Pozdnyakov, V.V. Korovushkin, A.M. Balagurov, I.A. Bobrikov, N. Fazel, M. Mouas, J.-G. Gasser, F. Gasser, P. Tabary, Q. Lan, A. Kovacs, S. Ostendorp, R. Hubek, S. Divinski, G. Wilde, Comparative study of structure and phase transitions in Fe-(25-27)% Ga alloys // Journal of Alloys and Compounds. - 2019. - 811. - 152030. doi:10.1016/j.jallcom.2019.152030.
15. I. Golovin, A. Balagurov, I. Bobrikov, S. Sumnikov, A. Mohamed, Cooling rate as a tool of tailoring structure of Fe-(9-33%)Ga alloys // Intermetallics. - 2019. - 114. - 106610. doi:10.1016/j.intermet.2019.106610.

16. M.V. Matyunina, M.A. Zagrebin, V.V. Sokolovskiy, O.O. Pavlukhina, V.D. Buchelnikov, A.M. Balagurov, I.S. Golovin, Phase diagram of magnetostrictive Fe-Ga alloys: insights from theory and experiment // Phase Transitions.- 2019. - 92. - 2. -P. 101-116. doi:https://doi.org/10.1080/01411594.2018.1556268.

17. N. Srisukhumbowornchai, S. Guruswamy, Influence of ordering on the magnetostriction of Fe-27.5at.%Ga alloys// Journal of Applied Physics. - 2002. - 92. - 9. - P. 5371-5379. doi:https://doi.org/10.1063/1.1508426.

18. T. V. Jayaraman, R. P. Corson, S. Guruswamy, Ordering, magnetostriction, and elastic properties in Fe-27.5at.% gaalloy single crystals // Journal of Applied Physics. - 2007. - 102. - 5. - 053905. doi:https://doi.org/10.1063/1.2777155.

19. G. Petculescu, K. L. Ledet, M. Huang, T. A. Lograsso, Y. N. Zhang, R. Q. Wu, M. WunFogle, J. B. Restorff, A. E. Clark, K. B. Hathaway, Magnetostriction, elasticity, and D 03 phase stability in Fe-Ga and Fe-Ga-Ge alloys // Jour- nal of Applied Physics. - 2011. - 109. - 7. - 07A904. arXiv:https://doi.org/10.1063/1.3535444, doi:10.1063/1.3535444. URL https://doi.org/10.1063/1.3535444

20. G. Petculescu, K. B. Hathaway, T. A. Lograsso, M. Wun-Fogle, A. E. Clark, Magnetic field dependence of galfenol elastic properties // Journal of Applied Physics. - 2005. - 97. - 10. - 10M315. doi:https://doi.org/10.1063/1.1855711.

21. R. Wu, Origin of large magnetostriction in FeGa alloys // Journal of Applied Physics. - 2002. - 91. - 10. - P. 7358-7360. doi:10.1063/1.1450791.

22. H. Wang, Y. N. Zhang, R. Q. Wu, L. Z. Sun, D. S. Xu, Z. D. Zhang, Understanding strong magnetostriction in fe100-xGax alloys // Scientific Reports. - 2013. - 3. -1. - P. 3521. doi:https://doi.org/10.1038/srep03521.

23. R. Wu, A. Freeman, Spin-orbit induced magnetic phenomena in bulk metals and their surfaces and interfaces // Journal of Magnetism and Magnetic Materials. - 1999. - 200. - 1. - P. 498-514. doi:10.1016/S0304- 8853(99)00351-0.

24. R. Wu, Z. Yang, J. Hong, First-principles determination of magnetic properties // Journal of Physics: Condensed Matter. - 2003. - 15. - 5. - P. S587-S598. doi:https://doi.org/10.1088/0953-8984/15/5/312.

25. Y. Zhang, R.Wu, Mechanism of large magnetostriction of galfenol // IEEE Transactions on Magnetics. - 2011. - 47. - 10. - P. 4044-4049. doi:10.1109/TMAG.2011.2158202.

26. D.S. Wang, R. Wu, A.J. Freeman, First-principles theory of surface magnetocrystalline anisotropy and the diatomic-pair model // Phys. Rev. B. - 1993. - 47. - P. 14932-14947. doi:10.1103/PhysRevB.47.14932. URL https://link.aps.org/doi/10.1103/PhysRevB.47.14932

27. G. Kresse, D. Joubert, From ultrasoft pseudopotentials to the projector augmented-wave method // Phys. Rev. B. - 1999. - 59. - P. 1758-1775. doi:10.1103/PhysRevB.59.1758.

28. G. Kresse, J. Furthmuller, Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set // Phys. Rev. B. - 1996. - 54. - P. 11169-11186. doi:10.1103/PhysRevB.54.11169.

29. J.P. Perdew, K. Burke, M. Ernzerhof, Generalized gradient approximation made simple [phys. rev.lett. 77, 3865 (1996)] // Phys. Rev. Lett. - 1997. - 78. - P. 1396-1396. doi:10.1103/PhysRevLett.78.1396.

30. K. Momma, F. Izumi, VESTA: a three-dimensional visualization system for electronic and structural analy- sis // Journal of Applied Crystallography. - 2008. - 41. - 3. - P. 653-658. doi:10.1107/S0021889808012016. URL https://doi.org/10.1107/S0021889808012016

31. V. Wang, N. Xu, J.C. Liu, G. Tang, W.-T. Geng, Vaspkit: A user-friendly interface facilitating highthrough- put computing and analysis using vasp code // Computer Physics Communications. - 2021. - 267. - P. 108033. doi:https://doi.org/10.1016/j.cpc.2021.108033.

32. Y.N. Lin, L.L. Li, X.-H. Yan, Y.P. Zhang, D.Y. Zhang, P. Zhang, Elastic and thermodynamic proper-ties of Fe3Ga from first-principles calculations // Solid State Communications. -

2016. - 230. - P. 43-48. doi:10.1016/j.ssc.2015.12.008.

33. Y.N. Zhang, R.Q. Wu, H.M. Schurter, A.B. Flatau, Understanding of large auxetic properties of iron-gallium and iron-aluminum alloys // Journal of Applied Physics. - 2010. - 108. - 2. - 023513. arXiv:https://doi.org/10.1063/1.3445269, doi:10.1063/1.3445269. URL https://doi.org/10.1063/1.3445269

34. X. Yan, Y. Lin, L. Li, F. Sun, Temperature-dependent elastic and thermodynamic properties of Fe 3 Ga (DO3, L12, and DO19) alloys from first-principles calculations // Physica status solidi (b). - 2016. - 253. - 11. - P. 2236-2244. doi:10.1002/pssb.201600314.

35. T.M. Inerbaev, A. Abuova, Y. Kawazoe, R. Umetsu, Local ordering and interatomic bond- ing in magnetostrictive Fe0:85Ga0:15X (X=Ni,Cu,Co,La) alloy // Computational Materi- als Science. - 2022. - 202. - 110934. doi:https://doi.org/10.1016/j.commatsci.2021.110934.

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Ga құрамының өзгеруімен D0 3 құрылымының Fe-Ga қорытпасындағы электронды құрылымның модификациясы және теріс магнитострикциясы

Аннотация. Ga құрамының өзгеруінің Fe_3Ga магнитострикциялық қасиеттеріне әсері. Тығыздықтың функционалдық теориясының әдістерімен $D0_3$ құрылымы бар қорытпа зерттелді. Зерттелетін қорытпаның стехиометриясының өзгеруі Fe атомдарын Ga-ға ауыстыру арқылы жүзеге асырылды. Ауыстыру зерттелетін жүйелердің электрондық құрылымының айтарлықтай өзгеруіне әкеледі, бұл Ферми деңгейіне жақын электрондық күйлердің тығыздығының айтарлықтай өсуіне әкеледі. Бұл әсер магнитті серпімділік энергиясының ұлғаюына әкеледі, бұл λ_{001} магнитострикциялық коэффициентінің мәнінің жоғарылауына әкеледі. Ары қарай λ_{001} ұлғаюы ығысу модулінің төмендеуіне байланысты болады, ол Ga құрамының ұлғаюымен жүйедегі бос байланыстар санының артуына байланысты болады. Нәтижесінде λ_{001} -дің Ga мазмұнына тәуелділігі, ол λ001 коэффициентінің абсолютті мәнінің жоғарылауын көрсетсе де, тәжірибеде байқалған магнитострикцияның оң шамасынан айырмашылығы оның теріс мәндерін береді. Магнитострикциялық коэффициенттердің теориялық және тәжірибелік мәндерінің белгісін сәйкестендіру мәселесін шешу қосымша зерттеулерді қажет етеді.

Түйін сөздер: Fe-Ga қорытпасы, электрондық құрылымы, тығыздықтың функционалдық теориясы, магнитострикция, магнитті серпімділік энергиясы.

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Модификация электронной структуры и отрицательная магнитострикция в сплаве Fe-Ga структуры D0₃ с изменением содержания Ga

Аннотация. Влияние изменения содержания Ga на магнитострикционные свойства Fe_3Ga. Сплав со структурой $D0_3$ исследовался методами теории функционала плотности. Изменение стехиометрии исследуемого сплава осуществлялось заменой Fe атомов на Ga. Замена приводит к существенному изменению электронной структуры исследуемых систем, что приводит к значительному увеличению плотности электронного состояния вблизи уровня Ферми. Этот эффект приводит к увеличению магнитоупругой энергии, что приводит к

увеличению значения магнитострикционного коэффициента λ_{001}. Дальше увеличение λ_{001} происходит за счет уменьшения модуля сдвига, которое происходит за счет увеличения числа рыхлых связей в системе с увеличением содержания Ga. Полученная зависимость λ_{001} от содержания Ga, хотя и показывает увеличение абсолютного значения коэффициента λ_{001}, дает его отрицательные значения, в отличие от положительной величины магнитострикции, наблюдаемой в эксперименте. Решение проблемы соответствия знака теоретических и экспериментальных значений магнитострикционных коэффициентов требует дальнейших исследований.

Ключевые слова: сплав Fe-Ga, электронная структура, теория функционала плотности, магнитострикция, магнитоупругая энергия.

References

1. E. Clark, K. B. Hathaway, Academic, San Diego, 1, 1 - 48 (2000).
2. E. du Tremolet de Lacheisserie, Springer-Verlag, New York, 213 - 234 (2005).
3. F. Jerems, C. M. Mahon, A. G. Jenner, R. D. Greenough, Amorphous magnetic materials for transducers, Ferroelectrics, 228 (1), 333 - 341 (1999). doi:https://doi.org/10.1080/00150199908226146.
4. J. D. Verhoeven, J. E. Ostenson, E. D. Gibson, O. D. McMasters, The effect of composition and magnetic heat treatment on the magnetostriction of TbxDy1xFey twinned single crystals, Journal of Applied Physics, 66 (2), 772 - 779 (1989). doi:https://doi.org/10.1063/1.343496.
5. J. Atulasimha, A. B. Flatau, A review of magnetostrictive iron-gallium alloys, Smart Materials and Structures, 20 (4), 043001 (2011). doi:10.1088/0964-1726/20/4/043001.
A. E. Clark, K. B. Hathaway, M. Wun-Fogle, J. B. Restorff, T. A. Lograsso, V. M. Keppens, G. Petculescu, R. A. Taylor, Extraordinary magnetoelasticity and lattice softening in bcc Fe-Ga alloys, Journal of Applied Physics, 93 (10), 8621-8623 (2003). doi:10.1063/1.1540130.
6. E. Clark, J. B. Restorff, M. Wun-Fogle, T. A. Lograsso, D. L. Schlagel, Magnetostrictive properties of body-centered cubic fe-ga and fe-ga-al alloys, IEEE Transactions on Magnetics, 36 (5), 3238-3240 (2000). doi:10.1109/20.908752.
7. Summers E. M., Lograsso T. A., Wun-Fogle M., Magnetostriction of binary and ternary Fe-Ga alloys, Journal of Materials Science, 42 (23), 9582-9594 (2007). doi:https://doi.org/10.1007/s10853-007-2096-6.
8. Q. Xing, Y. Du, R. McQueeney, T. Lograsso, Structural investigations of fe-ga alloys: Phase relations and magnetostrictive behavior, Acta Materialia, 56 (16), 4536-4546 (2008). doi:https://doi.org/10.1016/j.actamat.2008.05.011.
A. Clark, M. Wun-Fogle, J. Restorff, K. Dennis, T. Lograsso, R. McCallum, Temperature dependence of the magnetic anisotropy and magnetostriction of Fe100?xGax (x=8.6, 16.6, 28.5), Journal of Applied Physics, 97 (10, 3), 49th Annual Conference on Magnetism and Magnetic Materials, Jacksonville, FL, NOV 07-11, 2004 (MAY 15 2005). doi:10.1063/1.1856731.
9. W. Koster, T. Godecke, Uber den aufbau des systems eisen-gallium zwischen 10 und 50 at.-abhangigkeit von der warmebehandlung, International Journal of Materials Research, 68 (10), 661-666 (1977). doi:doi:10.1515/ijmr-1977- 681003
10. O. Kubaschewski, Iron-Binary phase diagrams, Springer Science & Business Media, 2013.
11. Golovin, A. Balagurov, V. Palacheva, A. Emdadi, I. Bobrikov, V. Cheverikin, A. Prosviryakov, S. Jalilzadeh, From metastable to stable structure: the way to construct functionality in Fe-27Ga alloy, Journal of Alloys and Compounds, 751, 364-369 (2018). doi:10.1016/j.jallcom.2018.04.127.
12. S. Golovin, A. K. Mohamed, V. V. Palacheva, V. V. Cheverikin, A. Pozdnyakov, V, V. V. Korovushkin, A. M. Balagurov, I. A. Bobrikov, N. Fazel, M. Mouas, J.-G. Gasser, F. Gasser, P. Tabary, Q. Lan, A. Kovacs, S. Ostendorp, R. Hubek, S. Divinski, G. Wilde, Comparative study of structure and phase transitions in Fe-(25-27)% Ga alloys, Journal of Alloys and Compounds, 811, 152030 (2019). doi:10.1016/j.jallcom.2019.152030.
13. Golovin, A. Balagurov, I. Bobrikov, S. Sumnikov, A. Mohamed, Cooling rate as a tool of tailoring structure of Fe-(9-33%)Ga alloys, Intermetallics, 114, 106610 (2019). doi:10.1016/j.intermet.2019.106610.

14. M.V. Matyunina, M.A. Zagrebin, V.V. Sokolovskiy, O.O. Pavlukhina, V.D. Buchelnikov, A.M. Balagurov, I.S. Golovin, Phase diagram of magnetostrictive Fe-Ga alloys: insights from theory and experiment, Phase Transitions, 92 (2), 101-116 (2019). doi:https://doi.org/10.1080/01411594.2018.1556268.

15. N. Srisukhumbowornchai, S. Guruswamy, Influence of ordering on the magnetostriction of Fe-27.5at.%Ga alloys, Journal of Applied Physics, 92 (9), 5371-5379 (2002). doi:https://doi.org/10.1063/1.1508426.

16. T. V. Jayaraman, R. P. Corson, S. Guruswamy, Ordering, magnetostriction, and elastic properties in Fe-27.5at.% ga alloy single crystals, Journal of Applied Physics, 102 (5), 053905 (2007). doi:https://doi.org/10.1063/1.2777155.

17. G. Petculescu, K. L. Ledet, M. Huang, T. A. Lograsso, Y. N. Zhang, R. Q. Wu, M. WunFogle, J. B. Restorff, A. E. Clark, K. B. Hathaway, Magnetostriction, elasticity, and D 03 phase stability in Fe-Ga and Fe-Ga-Ge alloys, Journal of Applied Physics, 109 (7), 07A904 (2011). arXiv:https://doi.org/10.1063/1.3535444, doi:10.1063/1.3535444. URL https://doi.org/10.1063/1.3535444

18. G. Petculescu, K. B. Hathaway, T. A. Lograsso, M. Wun-Fogle, A. E. Clark, Magnetic field dependence of galfenol elastic properties, Journal of Applied Physics, 97 (10), 10M315 (2005). doi:https://doi.org/10.1063/1.1855711.

19. R. Wu, Origin of large magnetostriction in FeGa alloys, Journal of Applied Physics, 91 (10), 7358-7360 (2002). doi:10.1063/1.1450791.

20. H. Wang, Y. N. Zhang, R. Q. Wu, L. Z. Sun, D. S. Xu, Z. D. Zhang, Understanding strong magnetostriction in fe100-xGax alloys, Scientific Reports, 3 (1), 3521 (2013). doi:https://doi.org/10.1038/srep03521.

21. R. Wu, A. Freeman, Spin-orbit induced magnetic phenomena in bulk metals and their surfaces and interfaces, Journal of Magnetism and Magnetic Materials, 200 (1), 498-514 (1999). doi:10.1016/S0304- 8853(99)00351-0.

22. R. Wu, Z. Yang, J. Hong, First-principles determination of magnetic properties, Journal of Physics: Condensed Matter, 15 (5), S587-S598 (2003). doi:https://doi.org/10.1088/0953-8984/15/5/312.

23. Y. Zhang, R. Wu, Mechanism of large magnetostriction of galfenol, IEEE Transactions on Magnetics, 47 (10), 4044-4049 (2011). doi:10.1109/TMAG.2011.2158202.

24. D.S. Wang, R. Wu, A. J. Freeman, First-principles theory of surface magnetocrystalline anisotropy and the diatomic-pair model, Phys. Rev. B, 47, 14932-14947 (1993). doi:10.1103/PhysRevB.47.14932.

25. G. Kresse, D. Joubert, From ultrasoft pseudopotentials to the projector augmented-wave method, Phys. Rev. B, 59, 1758-1775 (1999). doi:10.1103/PhysRevB.59.1758.

26. G. Kresse, J. Furthmuller, Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set, Phys. Rev. B, 54, 11169-11186 (1996). doi:10.1103/PhysRevB.54.11169.

27. J.P. Perdew, K. Burke, M. Ernzerhof, Generalized gradient approximation made simple [phys. rev.lett. 77, 3865 (1996)], Phys. Rev. Lett., 78, 1396-1396 (1997). doi:10.1103/PhysRevLett.78.1396.

28. K. Momma, F. Izumi, VESTA: a three-dimensional visualization system for electronic and structural analysis, Journal of Applied Crystallography, 41 (3), 653-658 (2008). doi:10.1107/S0021889808012016. URL https://doi.org/10.1107/S0021889808012016

29. V. Wang, N. Xu, J.C. Liu, G. Tang, W.-T. Geng, Vaspkit: A user-friendly interface facilitating highthroughput computing and analysis using vasp code, Computer Physics Communications, 267, 108033 (2021). doi:https://doi.org/10.1016/j.cpc.2021.108033.

30. Y.N. Lin, L.L. Li, X.-H. Yan, Y.P. Zhang, D.Y. Zhang, P. Zhang, Elastic and thermodynamic properties of Fe3Ga from first-principles calculations, Solid State Communications, 230, 43-48 (2016). doi:10.1016/j.ssc.2015.12.008.

31. Y.N. Zhang, R.Q. Wu, H.M. Schurter, A.B. Flatau, Understanding of large auxetic properties of iron-gallium and iron-aluminum alloys, Journal of Applied Physics, 108 (2), 023513 (2010). arXiv:https://doi.org/10.1063/1.3445269,

32. X. Yan, Y. Lin, L. Li, F. Sun, Temperature-dependent elastic and thermodynamic properties of Fe 3 Ga (DO3, L12, and DO19) alloys from first-principles calculations, physica status solidi (b), 253 (11), 2236-2244 (2016). doi:10.1002/pssb.201600314.

33. T.M. Inerbaev, A. Abuova, Y. Kawazoe, R. Umetsu, Local ordering and interatomic bonding in magnetostrictive Fe0:85Ga0:15X (X=Ni,Cu,Co,La) alloy, Computational Materials Science, 202, 110934 (2022). doi:https://doi.org/10.1016/j.commatsci.2021.110934.

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