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Magnetic properties and ferromagnetic materials describe the change of their shape or dimension in response to
the reorientation of magnetization under the influence of external magnetic field. Fe_{100-x}Ga_{x} alloys, binary alloys
(Galfenol) have large magnetostriction and excellent ductility; and they are very promising rare-earth free
materials for applications in sensors, actuators, energy-harvesters and spintronic devices. Here we report
results of large-scale ab initio molecular dynamics (AIMD) simulations for Galfenol, especially regarding
(Galfenol) result from intrinsic factors, namely, the Ga-induced changes of electronic structures. A major goal
of interdisciplinary research of Galfenol is to further enhance their magnetostrictive coefficients for robust
performance in devices. The abrupt drop of magnetostriction of Galfenol, at x ~ 19, a long-standing
puzzle for the community. Based on rigid band analysis, we propose possible ways to further optimize the
performance of Galfenol for device applications. For example, we found that the substitution of a small
amount of Cu for Ga (1.6%) in certain configuration may double the magnetostriction of Galfenol.

Structural, magnetic and magnetostrictive properties of Galfenol were obtained by performing large-scale
ab initio molecular dynamics (AIMD) simulations, using the Vienna Ab-initio Simulation Package (VASP).
We successfully reproduced the experimental thermodynamic properties of Fe_{100-x}Ga_{x} systems, and explained the decrease of
magnetostriction of Galfenol, at x ~ 19, with the atomic structures produced by AIMD simulations and the Boltzmann statistics. Furthermore, we found that adding a small amount
of Cu may extend the ascending trend of magnetostriction of Galfenol, by introducing a small amount of appropriate elements and also by
stabilizing them in benign structures.

To illustrate the AIMD simulation procedure in the present studies, we use Fe_{91.25}Ga_{18.75} as an example. We set
up ten initial configurations, with chemically random distributions of 104 Fe atoms and 24 Ga atoms on the bcc
lattice sites, and first kept them in melting state at 2000 K for 15 picoseconds (ps). As displayed in Fig. 1(a) for one
configuration, the free energy of the system quickly converged to about −773 eV/cell after 0.5 picoseconds,
indicating its thermal equilibrium. The Ga-Ga radial distribution function (RDF, denoted as \(g(r)\)) and the snapshot of atomic arrangement in the insets of Fig. 1(a) exhibit features of the liquid phase at 2000 K. We then cooled the system down from 2000 K to 500 K, with a cooling rate of \(10^{12} \text{K/s}\) around the melting point where the free energy decreases abruptly as shown in Fig. 1(b). The atomic structure at 500 K was further optimized at 0 K, with stringent criteria that require (1) force on each atom less than 0.01 eV/Å; (2) pressure along each axis smaller than 1.0 GPa, and (3) energy convergence better than \(10^{-5}\) eV.

Note that the calculated Ga-Ga RDF and snapshot of atomic arrangement in the insets in Fig. 1(b) show recrystallization of Galfenol at 500 K. It is important to point out that the number of Ga-Ga first neighbors is negligible in most structures obtained through our AIMD simulations. This is in good agreement with experimental observations that Ga and other metalloid atoms tend not to form first neighbors in the Fe matrix. The sharp peaks in the Ga-Ga RDF curve at 2.85 Å and 4.05 Å correspond to the B2-like and D0\(_1\) local structures, respectively. For comparison, the Ga-Ga RDF of the bulk D0\(_1\) structure was also given in the dashed line in the upper-left inset of Fig. 1(b).

To directly compare magnetostrictive coefficients and other quantities with experimental data, we calculated their ensemble averages for each Ga concentration according to

\[
(Q) = \frac{\sum_{n=1}^{N} Q_n \exp\left(E_n/k_B T\right)}{\sum_{n=1}^{N} \exp\left(E_n/k_B T\right)}
\]

Here, \(N\) is the number of configurations in the ensemble for each Ga concentration \((N = 10 \text{ in the present studies})\) and \(E_n\) and \(Q_n\) are total energies and the physical quantities of different configurations respectively. As an illustration, the calculated \(E_n\) and \(Q_n\) \((<\epsilon'>, <\epsilon'\text{b}_{1}>\) and \(<\lambda_{001}>\)) for ten different configurations of \(\text{Fe}_{81.25}\text{Ga}_{18.75}\) were presented in Table S1 in the Supplementary Materials. It is easy to see that the physical quantities are sensitive to the change of atomic structure at this Ga concentration. Since contributions from many configurations that have energies more than 400 meV higher than that of the best configuration are negligible due to their Boltzmann factors, we didn’t calculate their magnetoelastic responses.

For the determination of tetragonal magnetostriction coefficient, the supercells were deformed from their optimized geometries along the z-axis with the constant-volume mode \((\epsilon_x = \epsilon_y = -\epsilon_z/2)\). All atomic positions are further relaxed for each \(\epsilon_\text{z}\), \(\lambda_{001}\) for each configuration was calculated from the \(\epsilon_\text{z}\)-dependent total energy \(E_{\text{Total}}\) and magnetocrystalline anisotropy energy \(E_{\text{MCA}}\) according to the following formula\(^{19,20}\),

\[
\lambda_{001} = \frac{2dE_{\text{MCA}}/d\epsilon_\text{z}}{3dE_{\text{Total}}/d\epsilon_\text{z}^2} = -\frac{b_1}{3c}
\]

Here, the numerator and denominator are directly linked to the magnetoelastic coupling coefficient \((-b_1 = \frac{2}{3V_0} dE_{\text{MCA}}/d\epsilon_\text{z})\) and the tetragonal shear modulus \((c' = \frac{c_{11} - c_{12}}{2} = \frac{1}{2} \frac{d^2E_{\text{Total}}}{d\epsilon_\text{z}^2})\), respectively.

In particular, values of \(E_{\text{MCA}}\) are calculated by using the torque method, which was recently adapted to VASP\(^{21,22}\). To show the quality of our results, the calculated \(\epsilon_\text{z}\)-dependent \(E_{\text{Total}}\) and \(E_{\text{MCA}}\) for a configuration of \(\text{Fe}_{81.25}\text{Ga}_{18.75}\) are presented in the inset of Fig. 2(a). It is obvious that data points are smooth for high-quality fittings by polynomials of \(\epsilon_\text{z}\) (linear function for \(E_{\text{MCA}}\) and cubic function for \(E_{\text{Total}}\)). We determined \(<b_{1}>\), \(<c'>\) and \(<\lambda_{001}>) from the derivatives according to Eqs. (1) and (2) and the curve of \(<\lambda_{001}>) \sim x (0 \leq x < 21)\) is given in Fig. 2(a) (a factor of 3/2 was multiplied for easy comparison with experimental data). As found in experimental results\(^7\), \(<\lambda_{001}>) increases quadratically with x till \(x = \sim 19\) and decreases abruptly afterward. Fig. 2(b) shows that results of \(<b_{1}>\) and \(<c'>\) also agree well with their experimental counterparts: \(<c'>\) decreases linearly with x, while \(<b_{1}>\) peaks at \(x \sim 12.5\). These good agreements in a broad range of x suggest the validity and predictability of our theoretical approaches and models.

According to Eq. (2), an essential feature of strong magnetostrictive materials is having large \(E_{\text{MCA}}\) under a small lattice distortion. One factor for the enhancement of magnetoelastic coupling of Galfenol is that Ga atoms produce non-bonding Fe d-states in the minority spin channel. For 3d transition metal systems, the spin-orbit coupling Hamiltonian, \(H_{\text{SOC}} = \xi (\sigma \cdot L)\) with \(\sigma\) and \(L\) the spin and angular moment operators, is much weaker than their crystal fields (e.g., \(\xi\) is about 30 meV for Fe). The value of \(E_{\text{MCA}}\) can be reasonably estimated through the second order perturbation equation\(^{23}\),

\[
E_{\text{MCA}} = -\left(\frac{\xi}{2}\right)^2 \sum_{\sigma} \sum_{u} \frac{|\langle u | \sigma L | \phi \rangle|^2}{E_u - E_\phi}
\]
where $|\psi\rangle$ and $|\mu\rangle$ denote the occupied and unoccupied electronic states; and $E_\alpha$ and $E_b$ are their corresponding energies. For states close to the Fermi level, their SOC interactions with other states are strong because of the small denominators in Eq. (3), and also they are more responsive to lattice strain.

The existence of non-bonding Fe $d$-states is displayed by the curves of projected density of states (PDOS) in the inset in Fig. 2(c) for two Fe atoms (Fe$_1$ represents the first neighbors of Ga and Fe$_2$ represents the second neighbors of Ga) in Fe$_{81.25}$Ga$_{18.75}$. In contrast to the clear separation between the “bonding” and “antibonding” states for the bulk Fe (shaded background) and Fe$_2$ in the minority spin channel, high peaks of PDOS can be found around the Fermi level for the Fe$_1$ atom. These states have the $d_{x^2-y^2}$ feature, with their lobes pointing toward the first neighbors, and they become dangling bonds due to the weak Fe-Ga hybridization. A more clear demonstration of their wave function features can be found in Figure S1 in the Supplementary Materials for Fe$_{81.25}$Ga$_{18.75}$. The inset shows Fe$_{79.7}$Ga$_{20.3}$ that has a concentration of Ga slightly behind $x = 12.5$ which has also been observed by experimental detections. The coincidence between the drop of $<b_1>$ and the formation of D0$_3$-pairs indicates the detrimental effect of the D0$_3$ ordering on magnetostriction. Furthermore, the presence of B2-pairs appears not to have particular role for the enhanced magnetostriction of Galfenol up to $x = 19$.

One may use the rigid band model to analyze how $\lambda_{001}$ changes with the number of electrons in the unit cell ($N_e$)\textsuperscript{13,19}. The $E_{\text{MCA}}(N_e)$ curves of Fe$_{79.7}$Ga$_{20.3}$ that has a concentration of Ga slightly behind the drop of $<\lambda_{001}>$ are given in Fig. 3(a) with $\varepsilon_z = \pm 1\%$. Corresponding to the large decrease of $\lambda_{001}$ from $x = 19$ to $x = 20.3$, the value of $E_{\text{MCA}}$ for either $+1\%$ or $-1\%$ is small at $N_e = 1154$ (the number of valence electrons of 102 Fe and 26 Ga atoms). Interestingly, the two $E_{\text{MCA}}(N_e)$ curves with $\varepsilon_z = \pm 1\%$ actually cross each other near $N_e = 1154$. Therefore, one may enhance magnetostriction of Fe$_{79.7}$Ga$_{20.3}$ by either decreasing $N_e$ for positive $\lambda_{001}$, by replacing some Ga atoms with Cu or Zn atoms) or increasing $N_e$ (for negative $\lambda_{001}$, by replacing some Ga atoms with Ge atoms). Unfortunately, both Cu and Zn have poor solubility with Fe\textsuperscript{26}, so it might be a technical challenge to incorporate them uniformly in the FeGa lattice. For this reason, our AIMD simulations with the 128-atoms supercell indicate that Fe-Ga-Cu compounds don’t recrystallize at 500 K after the annealing/quenching procedure. To demonstrate the concept, we calculated magnetostrictive coefficients of three handpicked Fe-Ga-Cu configurations, which cover the most representative local structures. Interestingly, if we replaced two Ga atoms in Fe$_{79.7}$Ga$_{20.3}$ by Cu to form a hypothetical Fe$_{79.7}$Ga$_{18.7}$Cu$_{1.6}$ structure as depicted in the inset of Fig. 3(b), the calculated $\lambda_{001}$ can be as large as 550 ppm. The corresponding $-b_1$ is also large, 14.5 MJ/m$^3$, as shown by the brown filled circles at $x = 20.3$ for D0$_3$ phases.

![Figure 2](https://example.com/image2.png)  
**Figure 2** (Color online) (a) Calculated (red filled circles) x-dependent of $3/2<\lambda_{001}>$, along with the experimental data measured for the quenched samples at room temperature (dark cyan open circle)\textsuperscript{7}. The golden filled circle at $x = 20.3$ represents result for a metastable structure of Fe$_{79.7}$Ga$_{18.7}$Cu$_{1.6}$. The inset shows the strain-dependent total energy and magnetocrystalline anisotropy energy for one configuration of Fe$_{81.25}$Ga$_{18.75}$. (b) Calculated x-dependent $<c'>$ (red filled circles) and $<b_1>$ (blue filled circles), along with experimental data of $c'$ (open red circles and triangles) and $b_1$ (blue open circles)\textsuperscript{23,24}. The golden filled circle represents the calculated $b_1$ of a metastable structure of Fe$_{79.7}$Ga$_{18.7}$Cu$_{1.6}$. (c) Calculated x-dependent number of electronic states at the Fermi level in the minority spin channel, $N(E_{\text{F},\uparrow})$ (red filled circles), along with experimental data of $c$ (open red circles and triangles) and $b_1$ (blue open circles)\textsuperscript{23,24}. The golden filled circle represents the calculated $b_1$ of a metastable structure of Fe$_{79.7}$Ga$_{18.7}$Cu$_{1.6}$. (d) Number of D0$_3$ (black open circles) and B2 (x×30, purple filled circles) pairs. The insets show Fe (golden balls) and Ga (green balls) atoms in the D0$_3$ and B2 structures.

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The substitution of 1.6% Cu for Ga doesn't significantly affect the band structure around the Fermi level. These results show the importance of manipulating number of electrons for the design of new generation rare-earth-free magnetostrictive materials.

To further appreciate the effect of Cu on the electronic structures of Galfenol, the charge density difference, i.e., \( \rho(\text{Fe}_{79.7}\text{Ga}_{20.3}) - \rho(\text{Fe}_{79.7}\text{Ga}_{20.3}) \), was shown in Fig. 3(c). One may see that the effect of Cu in the Fe-Ga matrix is mainly localized around Cu and Fe\(_{1,Cu}\) (the nearest neighboring Fe atom to Cu) atoms. From the PDOS curves of Fe\(_{79.7}\text{Ga}_{20.3}\) in Fig. 3(d), we can see that the PDOS of Fe\(_{1,Cu}\) is not much different from that of Fe\(_{1,Ga}\). Both of them have fully occupied 3d bands in the majority spin channel and pronounced peaks of non-bonding \( d_{z^2} \) states near the Fermi level in the minority spin channel, as highlighted by the arrow. This suggests the similarity of Cu and Ga from the point view of their Fe neighbors. The bonding and anti-bonding states of the Fe\(_2\) atoms, the second neighbors to Cu and Ga, are well separated in energy in the minority spin channel, as for the binary Fe\(_{79.7}\text{Ga}_{20.3}\) alloy. The weak hybridization between d-states of Fe and Cu is also reflected in the curves of PDOS of Cu atoms in Fe\(_{79.7}\text{Ga}_{18.7}\text{Cu}_{1.6}\). The d-bands of Cu exist in a narrow range from \(-5\) to \(-3\) eV. Nevertheless, small tails of Cu d-states can be found around the Fermi level, which is not found for Ga atoms.

For experimental verifications, one needs to be cautious since the nonbonding states of Fe\(_{1,Ga}\) and Fe\(_{1,Cu}\) atoms.

\( \lambda_{001} \) in Fig. 2(a) and for \(-b_1\) in Fig. 2(b). Accordingly, the slope of strain dependent magnetocrystalline energy for Fe\(_{79.7}\text{Ga}_{20.3}\) is significantly larger than that for Fe\(_{79.7}\text{Ga}_{20.3}\) in Fig. 3(b). The calculated \( E_{\text{MCA}}(N_e) \) curves of the hypothetical ternary alloy with \( \epsilon_0 = \pm 1\% \) in Fig. 3(a) are similar with those of Fe\(_{79.7}\text{Ga}_{20.3}\), indicating that the substitution of 1.6% Cu for Ga doesn’t significantly affect the band structure around the Fermi level. These results show the importance of manipulating number of electrons for the design of new generation rare-earth-free magnetostrictive materials.

In conclusion, ab initio molecular dynamics simulations for Fe\(_{100-x}\text{Ga}_x\) binary and ternary alloys (0 \( \leq x \leq 21\)) revealed the mechanism for the drop of tetragonal magnetostriction \( \lambda_{001} \) at \( x = 19 \) and, more importantly, conceptually provided insights for avoiding the drop. As an example, we demonstrated that uniform substitution of a small amount of Cu for Ga might extend the rising trend of \( \lambda_{001} \) and double the magnetostriction of Galfenol, if appropriate metastable structures can be stabilized. This shows a new possibility to further optimize the performance of transition metal magnetostrictive alloys for practical applications.

**Methods**

Density functional simulations were performed with the Vienna Ab-initio Simulation Package. The exchange and correlation interactions among electrons were described at the level of the spin-polarized generalized gradient approximation (GGA), using the Perdew-Burke-Ernzerhof (PBE) functional\(^2\). We treated Fe-3d4s4p, Ga-3d4s4p and Cu-3d4s as valence states and adopted the projector-augmented wave (PAW) pseudopotentials to represent the effect of their ionic cores. Self-consistent calculations were performed in the non-collinear mode with the spin-orbit coupling (SOC) term\(^3\). The energy cutoff for the plane-wave expansion was 400 eV, sufficient for Fe-Ga systems according to our test calculations. A 4 \( \times \) 4 \( \times \) 4 cubic supercell (128 atoms/cell) was used to determine the chemical ordering of Ga in Fe\(_{100-x}\text{Ga}_x\).
alloys. While we used the Γ point to sample the Brillouin zone in the AIMD simulations, all geometries were further optimized with $5 \times 5 \times 5$ Monkhorst-Pack k-points before the determination of electronic and magnetic properties.

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Author contributions
H.W. and Y.N.Z. performed calculations. H.W. prepared the figures. H.W., Y.N.Z., L.Z.S. and R.Q.W. wrote the manuscript. D.S.X. and Z.D.Z. discussed results with others. All authors reviewed the manuscript. R.Q.W. supervised the project.

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