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Correlation of magnetocrystalline anisotropy of $Fe_{0.5}Pd_{0.5}$ alloy with chemical order

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Abstract
We study the magnetocrystalline anisotropy of $Fe_{0.5}Pd_{0.5}$ alloy using the first-principles spin-polarized relativistic Korringa–Kohn–Rostoker coherent-potential approximation. We investigate the effect of long-ranged chemical order on the magnitude as well as the direction of easy magnetization. We find that in this alloy, the chemical order enhances the magnitude of the magnetocrystalline anisotropy energy as well as altering the easy axis. In particular, for the $L1_0$ ordered alloy the easy axis is perpendicular to the alternating layers of Fe and Pd with quite large magnetocrystalline anisotropy energy 124 μeV. These observations are in very good agreement with experiments. We also find that it is the electronic structure in the vicinity of the Fermi surface that is responsible for this effect.

1. Introduction

In recent years, owing to the technological implications for high-density magneto-optical storage media [1, 2], there has been great interest in the magnetocrystalline anisotropy of ferromagnetic materials containing transition metals particularly in multilayered and thin-film form. For magneto-optical information storage and retrieval applications, films are required to exhibit perpendicular magnetic anisotropy (PMA), i.e. with the preferential direction of magnetization perpendicular to the film plane. In films, the 'effective' magnetic anisotropy constant, K_{eff}, follows an empirical relation:

$$K_{eff} = K_v + 2K_s/d$$

where K_v is the volume magnetic anisotropy constant, K_s is the surface magnetic anisotropy constant which arises due to the difference of the anisotropy of the interface atoms with respect to the inner or bulk atoms, and d is the thickness of the film. Clearly, the PMA is a result of play-off between K_v and K_s for a given thickness d of the film. K_v contains the volume magnetocrystalline anisotropy contribution, K, as well as the shape anisotropy contribution or the demagnetization energy given by $2\pi M_s^2$, where M_s is the saturation magnetization [2]. The magnetocrystalline anisotropy constant also determines the size of the magnetic domains, the domain wall thickness being inversely proportional to the magnetocrystalline anisotropy constant. K and M_s, and therefore K_v, are intrinsic properties of the materials. Therefore, *tailoring* magnetic materials with desired properties would require a knowledge of all these parameters, in particular K, the magnetocrystalline anisotropy energy (MAE).

The origin of magnetocrystalline anisotropy is the spin–orbit coupling [3] which is a relativistic phenomenon [4]. Also, experimental observations on ferromagnetic alloys indicate that there is a strong correlation between compositional order and magnetocrystalline anisotropy [5–13]. Recently [14–16], we presented a 'first-principles' theory of the magnetocrystalline anisotropy and its dependence on the atomic short-range order (ASRO) within the framework of spin-polarized relativistic Korringa–Kohn–Rostoker coherent-potential approximation [17] (SPR-KKR-CPA). We calculated the MAE of $\mathrm{Co}_c\mathrm{Pt}_{1-c}$ and $\mathrm{Fe}_c\mathrm{Co}_{1-c}$ alloys for various equilibrium as well as hypothetical compositional orders and found a strong correlation between the ASRO and MAE. Also, we produced the first quantitative explanation of the phenomenon of magnetic annealing [5, 6] in the permalloy.

Recently, there has been some interest in the magnetic anisotropy of $\mathrm{Fe}_{0.5}\mathrm{Pd}_{0.5}$ alloy films because these films exhibit a PMA comparable to that of CoPt alloy films as well as Co/Pt multilayers [11, 18, 19], and therefore may represent a low-cost alternative for magneto-optical storage devices. Below 920 K, the disordered bulk $\mathrm{Fe}_{0.5}\mathrm{Pd}_{0.5}$ alloy orders into a CuAu-type $L1_0$ layered ordered structure [20] with alternating planes of Fe and Pd atoms. The disordered alloy exhibits very small, almost zero, magnetocrystalline anisotropy [8], while the ordered alloy exhibits a strong magnetocrystalline anisotropy with the easy axis along the c-axis [9]. Although, the ordered phase is tetragonal there is evidence that the enhancement of the MAE is related to the ordering rather than the tetragonal distortion. In a more recent experiment using the magnetic x-ray circular dichroism, Kamp *et al* [11] have shown that in thick films of these alloys the enhancement of MAE is also linked to the compositional ordering. Although there have been a few theoretical investigations of the MAE of the perfect $L1_0$ ordered tetragonal FePd alloy [21, 22], it is still not clear how the onset of compositional ordering affects the magnetocrystalline anisotropy of this alloy. In this paper, we calculate the MAE of disordered $\mathrm{Fe}_{0.5}\mathrm{Pd}_{0.5}$ alloy as well as investigating the effect of different kinds of ASRO on the direction as well as magnitude of the MAE. In particular, we find that the long-range-ordered $L1_0$ structure has a much enhanced MAE compared with other hypothetical ordered structures, and that the easy axis is along the layer stacking direction, in complete agreement with the experimental observations [8, 9]. We also show that the MAE enhancement is a Fermi surface effect.

The outline of the paper is as follows. In section 2, we briefly refer to the formulation and some numerical and technical details. Afterwards, we present our results in section 3 and finally in section 4 we draw some conclusions.

2. Theory

The formulation and the computational details are discussed in the earlier publications [14–16], and the reader may refer to these. Here we reproduce only some key equations. The MAE of a compositionally disordered alloy $\mathrm{A}_c\mathrm{B}_{1-c}$ in the presence of ASRO can be defined as the difference between the free energies of the system, $K(\alpha) = \mathcal{F}(\boldsymbol{e}_1) - \mathcal{F}(\boldsymbol{e}_2)$, where $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$ are the two magnetization directions and α is the ASRO parameter. $K(\alpha)$ is small compared to the magnitudes of $\mathcal{F}(e_{1(2)})$ and therefore can be written approximately as [16]

$$K(\alpha) = K_{CPA} - \frac{1}{2\beta}\frac{1}{V_{BZ}}\int \mathrm{d}\boldsymbol{q}\,\alpha(\boldsymbol{q}; \boldsymbol{e}_1)[S^{(2)}(\boldsymbol{q}; \boldsymbol{e}_1) - S^{(2)}(\boldsymbol{q}; \boldsymbol{e}_2)] \tag{1}$$

where K_{CPA} is the MAE of the randomly disordered alloy, $\beta = (k_B T)^{-1}$ with k_B as the Boltzmann constant, and $S^{(2)}(\boldsymbol{q}; \boldsymbol{e})$ is the Fourier transform of the 'direct correlation functions', $S^{(2)}_{ij}(\boldsymbol{e})$, defined as the second derivative of the electronic grand potential $\Omega(\{c_i\}; \boldsymbol{e})$ with respect to the site-dependent concentrations $\{c_i\}$, i.e.,

$$S^{(2)}_{ij}(\boldsymbol{e}) = -\left.\frac{\partial^2 \Omega(\{c_i\}; \boldsymbol{e})}{\partial c_i\, \partial c_j}\right|_{\{c_i = c\}}.$$

The ASRO parameter is then given by

$$\alpha(\boldsymbol{q}; \boldsymbol{e}) = \frac{\beta c(1-c)}{1 - \beta c(1-c)[S^{(2)}(\boldsymbol{q}; \boldsymbol{e}) - \Lambda_c(\boldsymbol{e})]}$$

where $\Lambda_c(\boldsymbol{e})$ is the Onsager cavity correction [16]. Also, the spinodal transition temperature, T_c, below which the alloy orders into a structure characterized by the wave-vector $\boldsymbol{q}_{max}$ ($S^{(2)}(\boldsymbol{q}; \boldsymbol{e})$ is maximal at $\boldsymbol{q} = \boldsymbol{q}_{max}$), is given by

$$T_c = \frac{c(1-c)[S^{(2)}(\boldsymbol{q}_{max}; \boldsymbol{e}) - \Lambda_c(\boldsymbol{e})]}{k_B}.$$

For alloys with long-range order, the MAE is given by [16]

$$K(\boldsymbol{q}) \approx K_{CPA} - \frac{1}{2}|c_{\boldsymbol{q}}|^2[S^{(2)}(\boldsymbol{q}; \boldsymbol{e}_1) - S^{(2)}(\boldsymbol{q}; \boldsymbol{e}_2)] \tag{2}$$

where $c_{\boldsymbol{q}}$ is the amplitude of the concentration wave with wave-vector $\boldsymbol{q}$ which characterizes the ordered structure. $S^{(2)}(\boldsymbol{q}; \boldsymbol{e})$ can be calculated from first-principles electronic structure methods, such as using the SPR-KKR-CPA, and the details are given in reference [16]. The technical and computational details are discussed in reference [14].

Also, in reference [16] we have outlined a scheme for investigating the electronic origin of the MAE and its enhancement by compositional order. We can write the direct correlation function $S^{(2)}(\boldsymbol{q}; \boldsymbol{e})$ and the compositional order-dependent MAE $K(\boldsymbol{q})$ in terms of a sum over the Matsubara frequencies [23], $\omega_n = (2n+1)\pi k_B T$:

$$S^{(2)}(\boldsymbol{q}; \boldsymbol{e}) = 2k_B T \sum_n \mathrm{Re}[F(\boldsymbol{q}, \nu + \mathrm{i}\omega_n; \boldsymbol{e})] \tag{3}$$

and

$$K(\boldsymbol{q}) = K_{CPA} - 2k_B T \sum_n \mathrm{Re}[F(\boldsymbol{q}, \nu + \mathrm{i}\omega_n; \boldsymbol{e}_1) - F(\boldsymbol{q}, \nu + \mathrm{i}\omega_n; \boldsymbol{e}_2)] \tag{4}$$

where ν is the chemical potential and $F(\boldsymbol{q}, \varepsilon; \boldsymbol{e})$ is an energy-dependent electronic structure quantity given by

$$F(\boldsymbol{q}, \varepsilon; \boldsymbol{e}) = \frac{1}{V_{BZ}}\int \mathrm{d}\boldsymbol{k}\, \mathrm{Tr}[\{X_\mathrm{A} - X_\mathrm{B}\}\{\tau(\boldsymbol{k}+\boldsymbol{q})\lambda(\boldsymbol{q})\tau(\boldsymbol{k}) - \tau^{00}\lambda(\boldsymbol{q})\tau^{00}\}].$$

Here, $X_{\mathrm{A\,(B)}} = [(t^{-1}_{\mathrm{A\,(B)}} - t_c^{-1})^{-1} + \tau^{00}]^{-1}$ are the CPA *extra* scattering matrices for scattering from sites occupied by A-type (B-type) atoms, with $t_{\mathrm{A\,(B)}}$ and t_c the single-site scattering matrices for A-type (B-type) atoms and the CPA effective medium respectively. Also,

$$\tau^{00} = \frac{1}{V_{BZ}}\int \mathrm{d}\boldsymbol{k}\, \tau(\boldsymbol{k})$$

where $\tau(\boldsymbol{k}) = [t_c^{-1} - g(\boldsymbol{k})]^{-1}$ with $g(\boldsymbol{k})$ being the KKR structure constants matrix, and $\lambda(\boldsymbol{q})$ is obtained by solving the equation

$$\lambda(\boldsymbol{q}) = (X_{\mathrm{A}} - X_{\mathrm{B}}) - X_{\mathrm{A}}\left[\frac{1}{V_{BZ}}\int \mathrm{d}\boldsymbol{k}\;\tau(\boldsymbol{k}+\boldsymbol{q})\lambda(\boldsymbol{q})\tau(\boldsymbol{k}) - \tau^{00}\lambda(\boldsymbol{q})\tau^{00}\right]X_{\mathrm{B}}.$$

Therefore, a plot $F(\boldsymbol{q}, \nu + \mathrm{i}\omega_n; \boldsymbol{e})$ as a function of complex energy along the imaginary axis perpendicular to the chemical potential ν will give insight into the electronic origin of $S^{(2)}(\boldsymbol{q}; \boldsymbol{e})$ and $K(\boldsymbol{q})$. If the main contributions to $S^{(2)}(\boldsymbol{q}; \boldsymbol{e})$ and/or $K(\boldsymbol{q})$ come from small Matsubara frequencies, then it is the electronic structure in the vicinity of the Fermi surface that is important.

3. Results and discussion

Experimentally, the disordered fcc $\mathrm{Fe_{0.5}Pd_{0.5}}$ alloy undergoes a phase transition to a CuAu-type $L1_0$ layered ordered structure below 920 K with alternating layers of Fe and Pd atoms perpendicular to the c-axis. The ordered alloy is tetragonal, with a c/a ratio of 0.94. The disordered alloy exhibits almost no magnetic anisotropy [8] because of its cubic symmetry. In the ordered phase, the MAE is quite large, ~85.7 μeV/atom [9, 10], with the easy axis along the c-axis.

Our calculated results are summarized in tables 1 and 2. From table 1 we note that the order–disorder transition temperature is 1532 K which is quite high compared to the experimental value of 920 K [20]. However, considering that ours is a mean-field approach, the comparison is reasonable. Nevertheless, we predict that the $L1_0$ structure is the equilibrium ordered state ($S^{(2)}(\boldsymbol{q})$ is maximal for the $\boldsymbol{q} = (100)$ family which correspond to the $L1_0$ structure).

Table 1. Direct correlation functions $S^{(2)}(\boldsymbol{q}; [001])$ of several compositionally modulated $\mathrm{Fe_{0.5}Pd_{0.5}}$ alloys characterized by concentration wave-vectors $\boldsymbol{q}$.

$\boldsymbol{q}$	Ordered structure	$S^{(2)}(\boldsymbol{q}; [001])$ (eV)	T_c (K)
(001)	[001]-layered $L1_0$	0.53	1532
(100)	[100]-layered $L1_0$	0.53	1532
$(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	[111]-layered $L1_1$	−0.06	
$(\frac{1}{2}01)$		0.23	
$(1\frac{1}{2}0)$		0.23	
$(10\frac{1}{2})$		0.23	

In figure 1 we show the spin-polarized electronic density of states (DOS) for Fe and Pd components in the disordered $\mathrm{Fe_{0.5}Pd_{0.5}}$ alloy. Our results are very similar to the recent results for the $L1_0$ ordered FePd alloy [22]. A large exchange splitting is observed in the DOS of the Fe component which gives rise to a large spin magnetic moment 2.86 μ_B and there is no exchange splitting in the DOS of the Pd component although there is some rearrangement of electronic states giving rise to a comparatively small spin magnetic moment 0.25 μ_B. One important observation is that the majority-spin bands of both Fe and Pd are almost completely filled and show a common band-like behaviour whereas the minority-spin bands present a split-band picture. Again the Pd minority-spin band is almost completely filled while the Fe minority-spin band is only half-filled with a large DOS at the Fermi energy. From a simple tight-binding analysis this would mean that the band energy of the minority-spin electrons

Table 2. Magnetocrystalline anisotropy energy of $K(\boldsymbol{q})$ for several compositionally modulated $\mathrm{Fe}_{0.5}\mathrm{Pd}_{0.5}$ alloys characterized by concentration wave-vectors $\boldsymbol{q}$. Here the $K(\boldsymbol{q})$ are calculated with respect to the reference system which has the magnetization along the [001] direction (i.e. $\boldsymbol{e}_1 = [001]$) of the crystal. Thus when $K(\boldsymbol{q}) < 0$ the easy axis is along [001] and when $K(\boldsymbol{q}) > 0$ the easy axis is along $\boldsymbol{e}_2$.

		$K(\boldsymbol{q})$ (μeV)		
$\boldsymbol{q}$	Ordered structure	$e_2 = [111]$	$e_2 = [100]$	Easy axis
(001)	[001]-layered $L1_0$	−82.9	−124.5	[001]
(100)	[100]-layered $L1_0$	41.7	124.5	[100]
$(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	[111]-layered $L1_1$	−63.5	0.0	[001]
$(10\frac{1}{2})$		45.3	67.6	[100]
$(1\frac{1}{2}0)$		−22.3		
$(\frac{1}{2}01)$		−22.3		

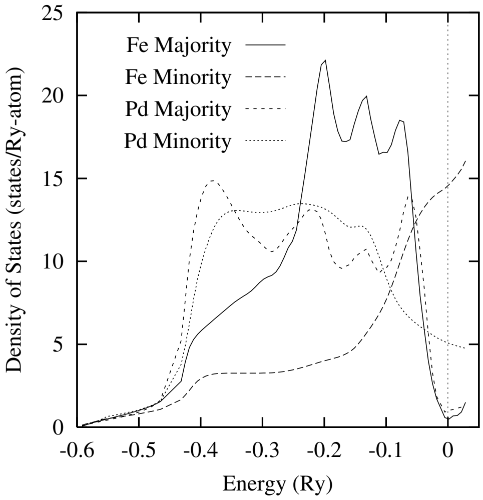

Figure 1. The spin-resolved local density of states of compositionally disordered fcc $\mathrm{Fe}_{0.5}\mathrm{Pd}_{0.5}$ alloy associated with the Fe and Pd sites. The energy is with respect to the Fermi energy.

would be lower if the constituent materials order whereas the majority-spin electrons will have negligible effect on this. Therefore, as in some other magnetic transition metal alloys [24], in the $\mathrm{Fe}_{0.5}\mathrm{Pd}_{0.5}$ alloy it is the minority-spin electrons which govern the ordering process.

In table 2 we show the results of magnetocrystalline anisotropy calculations for the observed ordered structure as well as some hitherto hypothetical ordered structures. We have calculated the MAE between the directions [001] and [111] as well as between [001] and [100]. Note that for a cubic symmetry case as in the disordered alloy, the MAE between [001] and [100] would be zero. For $\boldsymbol{q} = (001)$, i.e. when the layer stacking is along the [001] direction, we note that the easy axis is along the [001] direction, and for $\boldsymbol{q} = (100)$, i.e. for layer stacking along the [100] direction, the easy axis is along the [100] direction. This implies that for the $L1_0$ ordered structure the easy axis will always lie perpendicular to the layers of Fe and Pd. This is in complete agreement with the experimental observations. Also, the magnitude of the MAE between [001] and [111] directions (82.9 μeV) is in good agreement with the experimental value of 85.7 μeV [10].

Recently, Kamp *et al* measured the MAE of 300 Å thick [001]-oriented $Fe_{0.5}Pd_{0.5}$ films using magnetic circular x-ray dichroism and found that while the disordered film exhibits negligible magnetic anisotropy, the MAE increases as the chemical order η is increased. They quantify the chemical order η as the absolute value of the difference between the relative occupations of Fe atoms at the Fe and Pd sites, $\eta = |n_{\mathrm{Fe}} - n_{\mathrm{Pd}}|$, with $n_{\mathrm{Fe\,(Pd)}}$ determined by x-ray diffraction as described in reference [25]. Obviously, for a randomly disordered sample, $\eta = 0$, and for perfect $L1_0$ ordered sample, η should be equal to unity. According to this measurement, the MAE between the [001] and [100] directions for the most ordered film (with $\eta = 0.91$) is about 118 μeV which compares very well with our calculated value of 124.5 μeV for the perfect $L1_0$ ordered structure. Indeed, for $\eta = 0.91$ our estimation of the MAE is 105.4 μeV which is also in very good agreement with the result of Kamp *et al*. Ravelosona *et al* [26] also have measured the MAE of films of this type, but of thickness 1000 Å, so their results should be more like ones for bulk solids. They report the MAE to be 86 μeV for the $L1_0$ ordered sample with $\eta = 0.85$ which also compares well with our estimation of the MAE for $\eta = 0.85$ which is 90 μeV.

We have also calculated the MAE of some hitherto unfabricated hypothetical ordered structures as tabulated in table 2. The MAE for the hypothetical CuPt-type $L1_1$ layered ordered structure with the planes of Fe and Pd perpendicular to the [111] direction of the crystal is generated by a concentration wave-vector $\boldsymbol{q} = (\frac{1}{2}\frac{1}{2}\frac{1}{2})$. Unlike in the $Co_{0.5}Pt_{0.5}$ alloy, for which the MAE was largest for this structure [15, 16], in the $Fe_{0.5}Pd_{0.5}$ alloy the MAE is less than that of the $L1_0$ structure, and, more importantly, the easy axis is not perpendicular to the layer stacking; rather, it is along the [001] direction. Some other hypothetical structures described by the concentration wave-vectors $(10\frac{1}{2})$, $(1\frac{1}{2}0)$, and $(\frac{1}{2}01)$ which represent some kind of interdiffused layered structure [16] also exhibit quite small MAE values compared to the $L1_0$ structure. Very recently, Szunyogh *et al* [27] have calculated the magnetic anisotropy of ordered and disordered $Fe_{0.5}Pd_{0.5}$ alloy thin films from first-principles electronic structure calculations. They report that only the [001]-oriented $L1_0$ ordered structure exhibits PMA whereas the [111]-oriented ordered structure as well as the disordered and interdiffused layered structures do not show any PMA. The MAE of the [001]-oriented $L1_0$ ordered structure is around 60 μeV. Our results for the bulk alloy complement these results.

In order to probe the electronic origin of the structural ordering as well as the enhancement of the MAE in this alloy, we show plots of the real part of $F(\boldsymbol{q}, \varepsilon)$ and $\Delta F(\boldsymbol{q}, \varepsilon) = F(\boldsymbol{q}, \varepsilon; [001]) - F(\boldsymbol{q}, \varepsilon; [111])$ in figures 2 and 3 against the complex energy along the imaginary axis perpendicular to the Fermi level. It is quite clear from figure 2 that $F(\boldsymbol{q}, \varepsilon)$ has a long tail and that it has significant contributions coming from as far as 0.3 Ryd above the real axis. This means that in this alloy the ordering is not a Fermi surface effect. However, $\Delta F(\boldsymbol{q}, \varepsilon)$, as shown in figure 3, falls off rapidly as the imaginary part of the energy is increased, and it has significant contributions to the MAE only when the imaginary part is less than 0.15 Ryd. This implies that the MAE arises mainly from the electrons on or near the Fermi surface.

4. Conclusions

We studied the correlation between the magnetocrystalline anisotropy and chemical order in $Fe_{0.5}Pd_{0.5}$ alloy using the first-principles SPR-KKR-CPA electronic structure scheme. We found that when cooled from a high temperature, fcc $Fe_{0.5}Pd_{0.5}$ tends to order into a CuAu-type $L1_0$ layered ordered structure around 1532 K. In the $L1_0$ ordered alloy the magnitude of the MAE is 124 μeV and the easy axis of magnetization is perpendicular to the alternating planes of Fe and Pd. This is in very good agreement with experimental observations. Other

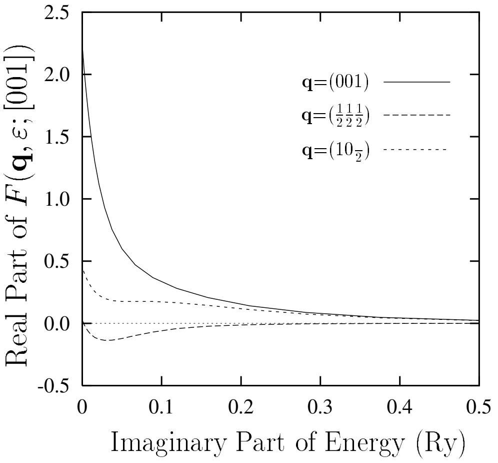

Figure 2. The real part of $F(\boldsymbol{q}, \varepsilon; [001])$ as given by (3) at complex energies along the imaginary axis perpendicular to the Fermi level for $\mathrm{Fe}_{0.5}\mathrm{Pd}_{0.5}$ alloy.

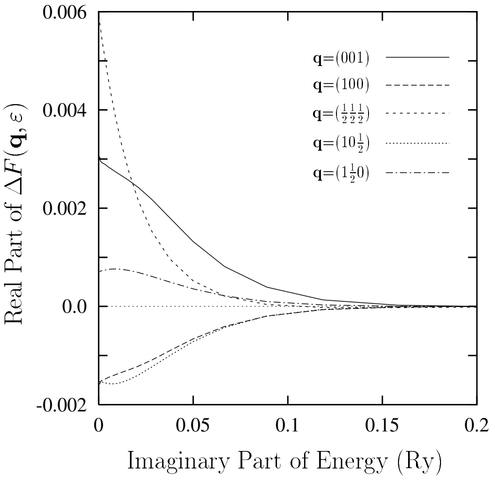

Figure 3. The real part of $\Delta F(\boldsymbol{q}, \varepsilon) = F(\boldsymbol{q}, \varepsilon; [001]) - F(\boldsymbol{q}, \varepsilon; [111])$, at complex energies along the imaginary axis perpendicular to the Fermi level for $\mathrm{Fe}_{0.5}\mathrm{Pd}_{0.5}$ alloy.

hypothetical ordered structures also exhibit an enhanced MAE, but the $L1_0$ ordered alloy has the largest MAE. A detailed investigation of the electronic structure and MAE reveals that it is the electronic structure in the vicinity of the Fermi surface that is responsible for the enhancement of the MAE in this alloy.

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