

Low stacking fault energy governs deformation mechanisms in the γ matrix of Co-based superalloys

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(Received 12 May 2026; revised 29 July 2026; accepted 23 September 2026; published 13 October 2026)

Understanding plastic deformation mechanisms in the γ matrix is essential for the development of next-generation Co-based superalloys. Since magnetic transitions in Co-based matrices can occur within service temperature ranges, stacking fault energies (SFEs) must be evaluated with explicit consideration of magnetic state effects. In this work, SFEs of pure Co and Co-rich alloys are calculated to quantify their compositional and temperature dependences in both ferromagnetic (FM) and paramagnetic (PM) states. The predicted values show good agreement with available experimental and theoretical data. For pure Co, the SFE increases with temperature in the FM state and decreases in the PM state; when the magnetic contribution is considered, the PM (Mag.) SFE exhibits the same trend as its FM counterpart. Co-rich alloys, by contrast, display a distinct temperature response, highlighting the dominant role of magnetic entropy in the PM state. Low SFEs predicted for Co-rich alloys at elevated temperatures favor deformation twinning, consistent with experimental observations. These results demonstrate that magnetic-state-dependent SFE calculations provide a robust framework for predicting plastic deformation modes and guiding the alloying design of Co-based alloys.

DOI: [10.1103/lzf5-2v51](https://doi.org/10.1103/lzf5-2v51)

I. INTRODUCTION

The γ' -hardened Co-based superalloys have gained significant attention due to their high strength and environmental resistance [1–3]. The ongoing development of alloys targets reduced density and improved thermodynamic stability through compositional optimization to achieve elevated-temperature performance that is competitive with Ni-base superalloys [2–7]. Due to the difference in lattice parameters between the γ matrix and the strengthening γ' precipitates, lattice misfits exist in superalloys—positive in Co-based [8] and mostly negative in Ni-based alloys [9]—which influence microstructure evolution and plastic deformation during creep and must therefore be considered in alloy analysis and design [2,8,10–12].

Despite compositional and microstructural differences, plastic deformation in both alloy families follows a general sequence. Dislocations are first activated in the softer γ matrix and glide on {111} planes under external stress. As dislocation

density accumulates, back stresses impede further passage through the matrix channels [12], and dislocation segments organize into interfacial networks at the γ/γ' boundaries. When applied and misfit stresses exceed a critical threshold, dislocations begin shearing into the γ' precipitates [2,10–12]. Importantly, even after deformation to plastic strains of $\sim 1.1\%$, the majority of deformation remains localized within the γ matrix [2,12], underscoring that the matrix governs the initial and dominant stage of deformation throughout the creep process.

The specific shearing mechanisms within γ' precipitates differ among alloy types: Co-based superalloys exhibit predominantly superlattice intrinsic and extrinsic stacking faults (namely, SISFs and SESFs) [2,3]; CoNi-base superalloys show antiphase boundaries (APBs) on {111} and {100} planes [13]; and Ni-base superalloys are governed by APB-coupled $a/2\langle 110 \rangle$ dislocation pairs. While extensive experimental [2,6–8,14,15] and theoretical [16,17] studies have focused on these γ' shearing mechanisms, the plastic deformation of the γ matrix from which all shearing dislocations originate has received comparatively limited systematic attention despite its key role in the initial stage of deformation [12,18,19].

Stacking fault energy (SFE) is a fundamental parameter governing plastic deformation in the fcc γ matrix. Plastic deformation proceeds through partial dislocation glide generating stacking faults (SF), deformation twinning (TW), and full dislocation slip (SL) [20–22], with the dominant

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mechanism determined by the magnitude of the SFE. The generalized stacking fault energy (GSFE) framework provides four key energy descriptors: unstable SFE (γ_{usf}), intrinsic SFE (γ_{isf}), unstable twinning fault energy (γ_{utw}), and stable twinning fault energy (γ_{tw}) that collectively define the energetic barriers for stacking fault formation and twin propagation [22–24]. Systematic investigation of these quantities across relevant alloy compositions is therefore essential for a physically rigorous understanding of γ matrix plasticity.

Further complexity in the γ matrix arises from elemental diffusion at elevated temperatures, which can induce local phase transformations [15], and from magnetic effects in alloy compositions where the Curie temperature (T_C) lies above room temperature [4,5]. Niu *et al.* demonstrated the coupling of chemistry and magnetism in CoCrNi alloys [25], and Oikawa *et al.* predicted a magnetically induced miscibility gap in Co-Cr alloys [26], indicating that magnetic contributions substantially influence both plastic deformation and phase stability. These findings establish that a comprehensive investigation of the SFE of the γ matrix accounting for alloy composition, temperature, and magnetic state is critically needed to advance the mechanistic understanding and computational design of next-generation Co- and Ni-base superalloys.

In this study, we calculate the composition and temperature effects on the SFE and lattice parameters (for lattice misfit) to understand dislocation dissociation mechanisms in the γ channel. The effect of temperature on these parameters is important because the plastic deformation processes of interest, such as creep, take place at high temperatures in superalloys. Accordingly, the GSFEs for pure Co, binary $\text{Co}_{1-x}\text{M}_x$ ($M = \text{W}, \text{Al}, \text{and Ni}$), and various Co-based alloys in ferromagnetic (FM) and/or paramagnetic (PM) states are calculated. Experiments are usually conducted at high temperatures above the Curie temperature T_C (e.g., 700°C–900°C), which necessitates a realistic description of the PM state in the DFT studies. In comparison, most of the previous theoretical works consider the situation in the FM state [16,17,25,27,28].

Since there are numerous experiments available on the plastic deformation of pure Co particularly at room temperature or above [20,26,29,30], it is a good starting point for Co-based alloys to study the plastic deformation behavior of pure Co and provide ideas for analyzing the possible deformation mechanism based on the predicted SFE value. Then we use the ternary composition of $\text{Co}_{81.7}\text{Al}_{9.3}\text{W}_9$ (at.%), the experimental measurement of the γ matrix of a dual-phase Co-based superalloy with a nominal alloy composition of Co-9W-9Al, to calculate the SFE and try to analyze the potential plastic deformation behavior. The composition of the γ matrix of dual-phase Co-based superalloys is always Co-rich. To investigate the complex chemical effect on the SFE, a series of CoCrNi-base alloys is also investigated and compared with existing experimental observations. To consider the temperature effects on plastic deformation, we further investigate two cases for Co-based alloys with multiphase or single-phase and calculate their SFE with temperature. They are commercial alloys MP35N with composition of $\text{Co}_{35.4}\text{Ni}_{35.5}\text{Cr}_{22.9}\text{Mo}_{6.2}$ [21] and commercial alloy SPRON510 with composition of $\text{Co}_{34}\text{Ni}_{31}\text{Cr}_{24}\text{Mo}_6\text{Fe}_2\text{Nb}_1\text{Ti}_1\text{Mn}_1$ [31]. These enable the further verification of the present theoretical work regarding

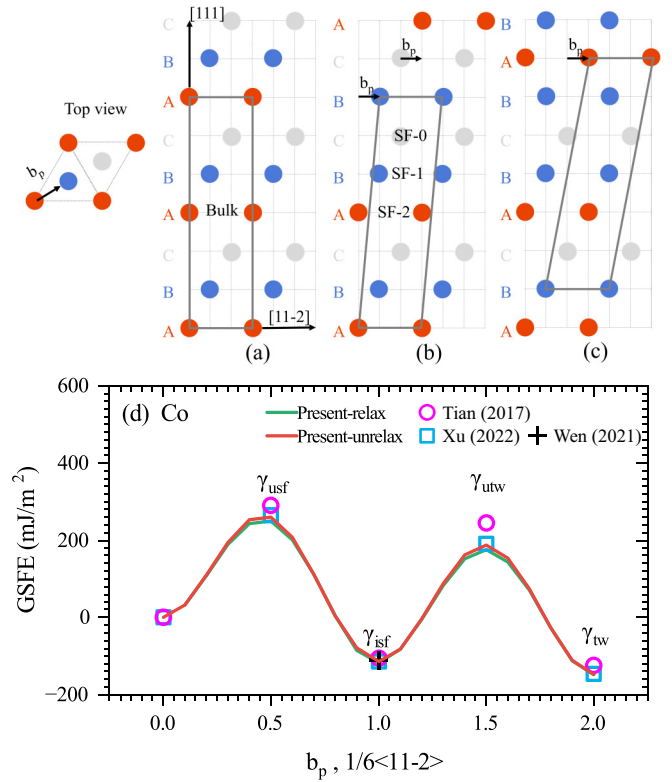


FIG. 1. Schematic of supercell (a $2 \times 2 \times 6$ unit cell) for GSFE calculations. (a) fcc perfect structure and (b) intrinsic stacking fault structure. The stacking fault layer is designated as SF-0, the first neighboring layer of the stacking fault is SF-1, and the second neighboring layer of the stacking fault is SF-2. (c) extrinsic stacking fault structure and (d) GSFEs of fcc Co at 0 K in the FM state with and without relaxations as a function of normalized displacement and compared with available theoretical data calculated by different methods [16,28,32]. The present results were obtained using the EMT0 method.

the prediction of plastic deformation mechanisms based on SFE values. Thus this work aims to predict the temperature-dependent plastic deformation behavior of the Co-based alloys or hard metals at the atomic level using a robust *ab initio* approach, and to provide the knowledge to facilitate the design of multi-component materials with tailored mechanical performance.

II. METHODOLOGY AND COMPUTATIONAL DETAILS

A. Generalized stacking fault energy (GSFE)

A supercell (SC) consisting of six $\{111\}$ slip planes was constructed to model structures with and without stacking faults. In an ideal fcc lattice, a full dislocation with Burgers vector $\mathbf{b}_1 = \frac{1}{2}[10\bar{1}]$ can energetically dissociate into two partial dislocations with Burgers vectors $\mathbf{b}_2 = \frac{1}{6}[11\bar{2}]$ and $\mathbf{b}_3 = \frac{1}{6}[2\bar{1}\bar{1}]$. Accordingly, tilt supercells containing a single stacking fault ($\dots\text{ABC}|\text{BCA}\dots$, where “|” marks the fault plane) were generated by rigidly shifting the upper half of the crystal relative to the lower part by a vector $\mathbf{x}$ of $\mathbf{b}_p = 1/6[11\bar{2}]$. Thus the GSFE is a function of the shift vector $\mathbf{x}$, as shown schematically in Figs. 1(a)–1(c). The actual SC used in this

work is a $2 \times 2 \times 6$ cell, meaning that in each close-packed layer there are four atoms. This allows for doping in a single layer.

Atomic relaxation along the $\langle 111 \rangle$ direction was not considered for any of the investigated systems except for pure Co at 0 K. As shown in Fig. 1, layer relaxation does not influence the overall conclusions for pure Co within this study, and therefore its effect is deemed negligible. For dilute Co-based alloys, the relaxation effect is similarly assumed to be minor and is therefore neglected. Based on this configuration, the characteristic fault energies, i.e., γ_{usf} (at $x = 0.5b_p$), γ_{isf} (at $x = 1.0b_p$), γ_{utw} (at $x = 1.5b_p$), and γ_{tw} (at $x = 2.0b_p$), were obtained using

$$\gamma(x) = \frac{E(x) - E(0)}{A}, \quad (1)$$

where $E(x)$ and $E(0)$ are the total energies of the defective and defect-free configurations, respectively, and A ($\sqrt{3}a_{\text{fcc}}^2$) is the area of the corresponding fault plane. It should be noted that the extrinsic stacking fault is generated on the pre-existing intrinsic stacking fault or twin fault.

Given that the predicted Curie temperature of the ternary $\text{Co}_{81.7}\text{Al}_{9.3}\text{W}_9$ alloy is approximately 596 K in this work using mean-field approximation [5], the PM SFE of this alloy was also evaluated. The magnetic entropy contribution to the SFE, γ_{mag} , was calculated using

$$\gamma_{\text{mag}}(x) = -\frac{T[S(x) - S(0)]}{A}, \quad (2)$$

where the magnetic entropy is approximated as $S(x) = k_B \sum c_i \ln(1 + \mu(x))$, with k_B being the Boltzmann constant, and c_i and $\mu(x)$ denoting the concentration and local magnetic moment of the magnetic atoms in a given configuration. $S(0)$ is the magnetic entropy of the ideal, defect-free configuration. This approach assumes a random local-moment description and neglects short-range magnetic correlations and spin fluctuations beyond the mean-field approximation as proposed by Grimvall [33]. This method has been applied in previous SFE calculations for many complex alloys [4,34,35]. Accordingly, the magnetic entropy contribution to the stacking fault energy occurs only when the local magnetic moment changes around the stacking fault. It should be noted hereinafter that PM SFE without magnetic entropy contribution is calculated according to Eq. (1). The PM SFE including magnetic entropy contribution is calculated according to Eqs. (1) and (2), and the results are referred to PM(Mag.).

Previous studies have shown that limiting the interlayer interactions to the first order within the so-called axial interaction model (AIM) provides a good approximation for the intrinsic SFE [28,34,36]. Therefore, for comparison, we also estimated the intrinsic stacking fault energy with a $1 \times 1 \times 1$ unit cell in the SC calculations by using $\gamma_{\text{isf}}^{\text{AIM}} = 2(E_{\text{hcp}} - E_{\text{fcc}})/A$, where E_{hcp} and E_{fcc} are the total energies per atom of the hexagonal close-packed (hcp) and fcc structures, respectively, and $A = \sqrt{3}a_{\text{fcc}}^2/4$ is the stacking fault area. The c/a ratio of the hcp structure is fixed at 1.63 in all calculations. This is supported by the fact that the interlayer distance near the stacking fault shows negligible relaxation, i.e., stays close to the ideal in-plane nearest-neighbor distance of 0.815.

B. Computational and numerical details

The exact muffin-tin orbitals (EMTO) method [37,38] combined with the coherent potential approximation (CPA) [39,40] was used for the *ab initio* calculations based on density functional theory. The full charge density method was applied for the calculation of the total energy [41]. We utilized the generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) functional [42] as the exchange-correlation functional for the self-consistent calculations. Both chemical and magnetic disorders were described using the CPA. The PM state was treated as a random spin state using the disordered local moments (DLM) scheme [43–45]. The k -point meshes were set to $29 \times 29 \times 29$ and $6 \times 11 \times 4$, respectively, to calculate the equilibrium lattice constant and GSFE of fcc cell and the supercell with and without a stacking fault. Convergence for both k -point mesh densities was carefully tested. In CPA calculations, we employed a screening parameter of 0.9, which is important in Co-based alloys [4,5]. The coherent potential approximation is a single-site impurity approximation, and therefore, no information is available about the charge distribution beyond the single impurity site. To remedy this problem, researchers introduced the so-called screened impurity model (SIM) [46], which is adopted here as well. We carried out several test calculations to see how sensitive the computed properties are to the screening parameter, which controls the electrostatic potential correction within the CPA-SIM scheme. The most critical case is the Co-W binary system, where results critically depend on the actual choice of the screening parameter. Comparing the total energy of a supercell (no CPA) with that of the CPA, we found that the optimal screening parameter is around 0.86. The tests can be found in Supplemental Material (SM) Fig. S1 [47]. These calculations were carried out at the equilibrium volume of Co. It should be noted that the results are insensitive to this parameter for the Co-Ni and Co-Al systems. Taking into account that the screening parameter slightly depends on volume and W addition to Co strongly increases the volume [48], we selected a constant screening parameter of 0.9 in all our EMTO-CPA calculations.

The Vienna *ab initio* simulation package (VASP) [49] in conjunction with the projector augmented-wave (PAW) [50] approach, using the same exchange-correlation functional and SC configuration as employed in EMTO, was adopted to calculate the SFE for comparison. The energy cutoff was set to 500 eV, and the k -point spacing in all three directions was $2\pi \times 0.03 \text{ \AA}^{-1}$ (i.e., Γ -centered k mesh is $8 \times 8 \times 3$ for the 24-atom SC) for all calculations. The convergence criteria for calculating the electronic energy and force were set to 10^{-6} eV and -0.01 eV/ $\text{\AA}$, respectively.

The temperature dependence of the lattice parameters was estimated by using a constant (temperature-independent) linear thermal expansion coefficient of Co ($\alpha_{\text{Co}} = 0.000013$ 1/K [51]), which gives a good description of the lattice constant of pure Co at elevated temperatures. Later, we used the corresponding lattice constant at each temperature to calculate the SFEs of pure Co and obtain the correlation between SFE and lattice constant ($\gamma_{\text{isf}} = 474.18a - 1788.8$, $R^2 = 0.998$, a in units of $\text{\AA}$, γ_{isf} in units of mJ/m^2). This relationship can be

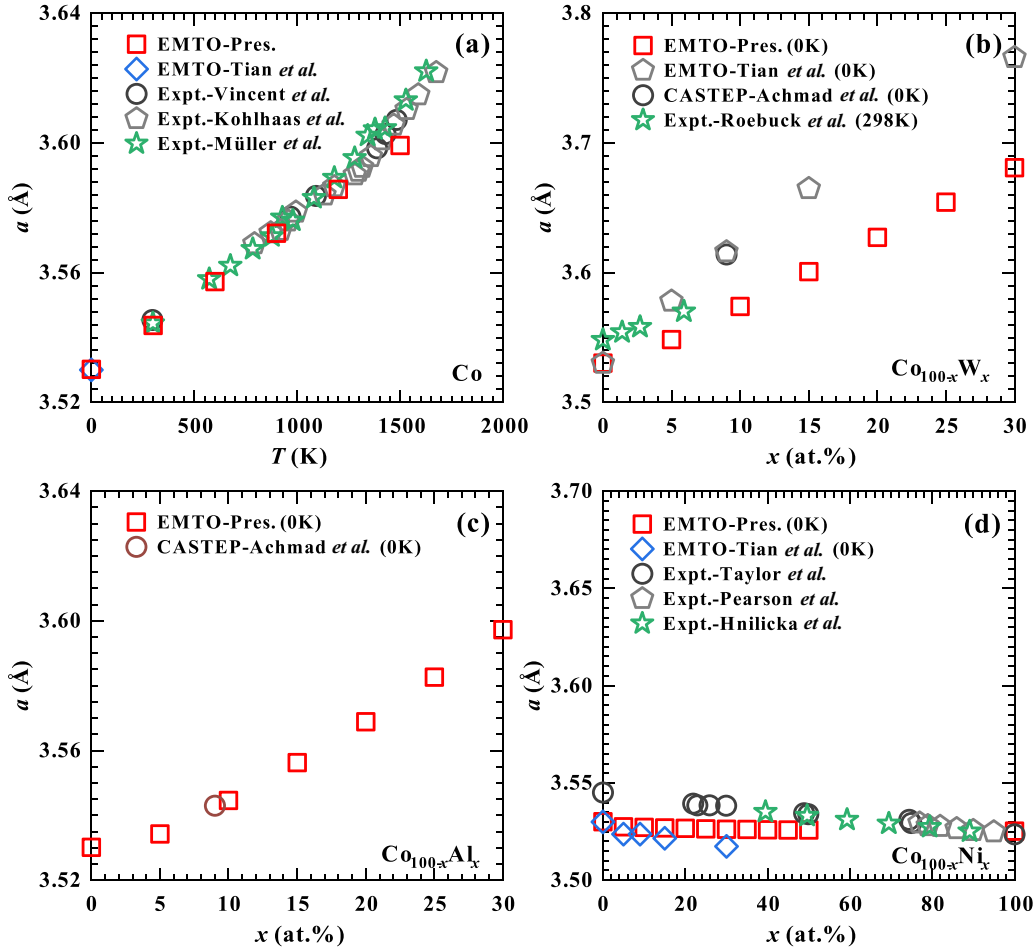


FIG. 2. Lattice constants for Co and binary Co-based alloys. (a) Temperature dependence of lattice constant for pure Co, (b) $\text{Co}_{100-x}\text{W}_x$, (c) $\text{Co}_{100-x}\text{Al}_x$, and (d) $\text{Co}_{100-x}\text{Ni}_x$ as a function of x , compared to the theoretical [28,53] and experimental data [52,54–62] from literature.

used to separate the chemical and volume effects for binary $\text{Co}_{100-x}\text{M}_x$ alloys. There are two ways to define the chemical effect. One way is to fix the lattice constant to that of pure Co at 0 K while changing the concentration of M. The other way is to use the results for the binary $\text{Co}_{100-x}\text{M}_x$ system and subtract the results of pure Co, which were calculated using the same individual lattice constant of the corresponding binary $\text{Co}_{100-x}\text{M}_x$ system. Here we only present the results for the second method. The temperature dependence of SFE for pure Co and ternary $\text{Co}_{81.7}\text{Al}_{9.3}\text{W}_9$ alloys was also considered by using the corresponding experimental lattice parameters at each temperature for *ab initio* calculations. That is, we only considered the contribution of the thermal expansion to the temperature effect. The lattice parameters are extracted from the previous experimental works [8,52].

III. RESULTS

A. Lattice constant

Figure 2 presents the lattice constants of pure Co as a function of temperature [Fig. 2(a)] and binary $\text{Co}_{100-x}\text{M}_x$ ($M = \text{W}, \text{Al}, \text{and Ni}$, respectively) systems as a function of concentration [Figs. 2(b)–2(d)]. We calculated the lattice parameter of Co at 0 K to be 3.530 Å, showing excellent agreement with other theoretical [28,63] and experimental

data at 300 K (3.544 Å) [52] with a deviation of less than 0.4%. The temperature-dependent lattice constant follows the experimental data, even though the increment is a little bit smaller than the experimental values at higher temperatures [Fig. 2(a)]. This slight underestimation of lattice expansion stems most probably from the use of a constant thermal expansion coefficient for the calculated lattice constants. Nevertheless, the calculated lattice constants show a satisfying alignment with the available experimental data [52,54–56]. The present temperature-dependent lattice parameter of Co will be used to consider the influence of temperature on SFE by accounting for the thermal lattice expansion.

When adding W, the lattice constant of the $\text{Co}_{100-x}\text{W}_x$ system increases with increasing W content, and it follows the same trend as the reference data [28,53,57] [Fig. 2(b)]. The lattice constants for $\text{Co}_{100-x}\text{W}_x$ calculated in the present work can be approximated by a linear regression function of $a_{\text{theo.}} = 0.0051x + 3.5253$ ($R^2 = 0.998$) (x is in at.%) and the experimental data by a function of $a_{\text{exp.}} = 0.0037x + 3.5483$ ($R^2 = 0.998$) [57]. For comparison, the literature theoretical data can be described by a function of $0.0078x + 3.5392$ ($R^2 = 0.992$) [28]. Although in that reference, researchers adopted the same method as here, they used a screening parameter of 0.6. It is interesting to note that the current EMTO results are much closer to the experimental data, even though

TABLE I. Theoretical SFE and lattice constants for pure Co in ferromagnetic and paramagnetic states. Shown are the lattice parameter a (in units of Å), the intrinsic and unstable SFE γ_{isf} , γ_{usf} determined using the supercell method (a $2 \times 2 \times 6$ unit cell), and the unstable and stable twin formation energies, γ_{utw} , γ_{tw} respectively. The results are compared to the first-order term in the axial interaction model (AIM) $\gamma_{\text{isf}}^{\text{AIM}}$, and available experimental [64] and theoretical [16,25,28,32,53] data, as shown in Table S1 [47]. γ_d is the deformation parameter proposed by Jo *et al.* [22] while τ_a represents the twinnability in fcc structure, as defined in Ref. [65].

Co	Magnetic state	T (K)	a (Å)	γ_{usf} (mJ/m ²)	γ_{isf} (mJ/m ²)	$\gamma_{\text{isf}}^{\text{AIM}}$ (mJ/m ²)	γ_{utw} (mJ/m ²)	γ_{tw} (mJ/m ²)	γ_d	τ_a	Method
	FM	0	3.530	260.5	-114.8	-107.3	187.6	-147.1	-0.31	1.02	EMTO
	PM	0	3.530	368.3	17.1		382.7	27.7	0.05	1.15	EMTO
	FM	300	3.544	253.3	-108.0		183.0	-141.0	-0.30	1.02	EMTO
	PM	300	3.544	352.8	14.4		365.0	25.0	0.04	1.15	EMTO
	FM	0	3.530	276.5	-111.0						VASP

the cited experimental data are measured at room temperature for Co-W alloys containing small amounts of C. We notice that carbon does not strongly influence the dependence of lattice constant on W content, which is demonstrated by Ref. [57]. The difference between the present and former theoretical results obtained with the EMTO method mainly stems from the different screening parameters used to correct the electrostatic energy within the single-site approximation. The screening parameter can make a significant difference for some alloys with transition metal W, which has been reported in our previous work as well [4,5].

The addition of Al increases the lattice constant of the Co_{100-x}Al_x system [Fig. 2(c)], showing good agreement with theoretical data computed using the CASTEP software [53]. The lattice constants of the Co_{100-x}Ni_x system decrease slightly with increasing Ni content [Fig. 2(d)] and by this show a similar trend as the experimental and theoretical data from the literature [28,59–61]. The experimental data of Jen *et al.* [62] and theoretical data of Tian *et al.* [28] also show a decrement of the lattice constant with increasing Ni content, which is slightly larger than the present results. However, the present calculated results with a screening parameter of 0.9 are slightly closer to other experimental data [52,59–61]. This indicates a good prediction capability for lattice constant calculations of alloys by the EMTO method if a proper screening parameter is used.

B. Chemical influence on stacking fault energy

In the following part, we present the generalized stacking fault energies for pure Co, binary Co- M ($M = \text{W, Al, and Ni}$) alloys, and ternary Co-Al-W alloys and investigate the variation of SFE with increasing volume (temperature) and chemical composition. The numerical results are presented in a series of tables, figures, and SM [47].

1. Pure Co

Figure 1 shows the GSFEs of pure Co as a function of displacement in the FM state, in comparison with other theoretical results from the literature [16,25,28,32,53]. The corresponding numerical values are listed in Tables I and S1 [47].

We calculate the γ_{isf} of FM Co using EMTO as -114.8 mJ/m² with the supercell method, which agrees well with the value of -111 mJ/m² obtained using VASP. Furthermore, the value also agrees well with previous DFT

calculations (-106.2 mJ/m² [28] using EMTO and values between -120 and -110 mJ/m² [16] using VASP). Adopting the first-order approximation of the AIM approach, the present value is -107.3 mJ/m², which is in good agreement with the value reported by Tian *et al.* (-105.6 mJ/m²) [28] calculated also using the AIM approach, indicating that with the current configuration of defects the theoretical calculations yield reasonable results. The available high-temperature experimental data extrapolated linearly give -50 mJ/m² at 0 K [28]. Thus there is a large deviation between the theoretical results and the estimated low-temperature experimental data. However, a linear extrapolation might not be adequate, as demonstrated in the case of fcc Fe [34]. Nevertheless, it is important to notice that even a simple linear extrapolation predicts negative SFE for pure fcc Co at 0 K.

In Table I, the FM γ_{usf} is 260.5 mJ/m² obtained with EMTO, and 276.5 mJ/m² computed by VASP. These values are smaller than the previously reported γ_{usf} using the same EMTO method (Refs. [28,32]), which might be due to the use of a $1 \times 1 \times 9$ supercell in those works. By comparing the two intrinsic energy barriers for stacking fault formation and twin formation, viz. γ_{usf} (260.5 mJ/m²) and $\gamma_{\text{utw}} - \gamma_{\text{isf}}$ (302.4 mJ/m²), respectively, one can deduce the activated deformation mechanism [22]. Accordingly, in pure Co, the formation of stacking faults during plastic deformation is predicted at low temperature.

Figure 3 presents the changes of the SFE and energy barriers with lattice constant in different states. One can see that FM γ_{isf} increases with lattice constant [Fig. 3(a)]. The lattice constants shown as red circles correspond to the temperatures marked in Fig. 3(b). In Fig. 3(b), both γ_{usf} and $\gamma_{\text{utw}} - \gamma_{\text{isf}}$ decrease with volume/temperature in FM state, implying that the positive barriers for the formation of stacking faults and twins decrease. Since γ_{usf} remains lower than $\gamma_{\text{utw}} - \gamma_{\text{isf}}$ at all volumes, we conclude that SF will form with increasing lattice constant/temperature. The negative $\gamma_{\text{utw}} - \gamma_{\text{usf}}$ displays a weak increase with lattice constant/temperature, showing that the decrease of γ_{usf} is more pronounced than that of γ_{utw} . We notice that the effective energy barrier for full slip, $\gamma_{\text{usf}} - \gamma_{\text{isf}}$ (Ref. [22], not shown), is the largest among the effective energy barriers at all volumes, indicating that full-slip is less feasible than stacking fault formation or twinning. The PM and PM(Mag.) results show similar trends for γ_{usf} and $\gamma_{\text{utw}} - \gamma_{\text{isf}}$ with lattice constant/temperature. PM γ_{usf} is slightly higher than PM $\gamma_{\text{utw}} - \gamma_{\text{isf}}$ in the range of 0–1200 K,

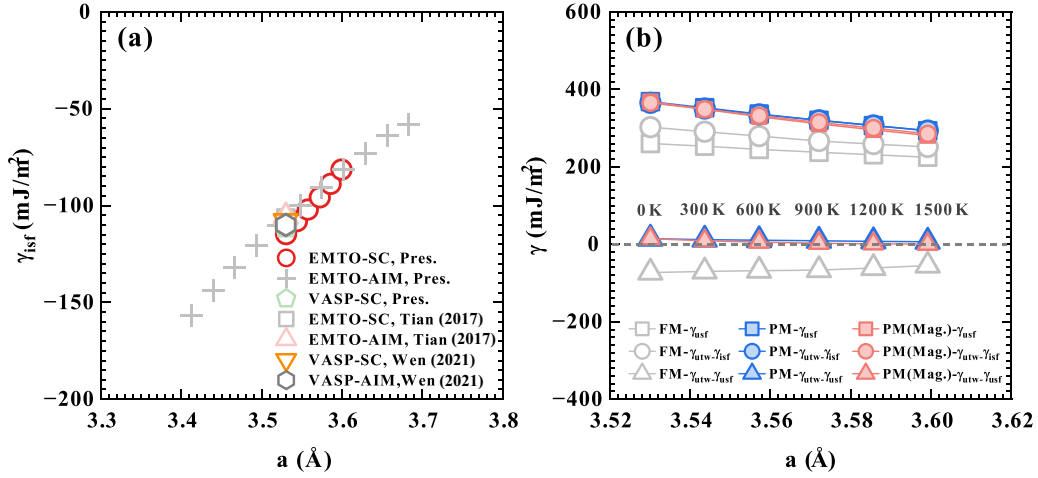


FIG. 3. Theoretical SFE of pure Co. (a) SFE of FM Co as a function of lattice constant, compared with theoretical data from the literature [16,28]. (b) The energy barriers for stacking fault formation (square symbol, γ_{usf}), twin formation (circle symbol, $\gamma_{\text{utw}} - \gamma_{\text{isf}}$) and energy difference ($\gamma_{\text{utw}} - \gamma_{\text{usf}}$) in unstable fault energies for FM (gray color), PM (blue color), and PM (Mag.) (red color) as a function of lattice constant. We used the linear thermal expansion method to extrapolate the lattice constants at finite temperature. The corresponding temperatures are marked in (b).

while PM(Mag.) γ_{usf} is slightly lower than PM(Mag.) $\gamma_{\text{utw}} - \gamma_{\text{isf}}$ in the range of 300–1500 K. Both PM and PM(Mag.) $\gamma_{\text{utw}} - \gamma_{\text{usf}}$ are positive and show a slight decrease with lattice constant/temperature. The change for PM(Mag.) $\gamma_{\text{utw}} - \gamma_{\text{usf}}$ with volume is slightly more pronounced than that of PM $\gamma_{\text{utw}} - \gamma_{\text{usf}}$, which implies the magnetic effect on the SFEs. We will come back to this point later.

2. Co-W binary alloys

Next, the alloying influence of W, Al, and Ni on the SFE of binary $\text{Co}_{100-x}\text{M}_x$ systems is investigated by using the EMT0 method. As experiments have found that heavy elements (such as W) could segregate at the stacking fault plane in Co-based alloys [3,6,66,67], the segregation of alloying elements at the stacking fault layer is also investigated.

Figure 4 shows the SFE of FM $\text{Co}_{100-x}\text{W}_x$ as a function of W concentration, and detailed values can also be found in Table S2 [47]. In general, the SFE of FM $\text{Co}_{100-x}\text{W}_x$ increases

at larger W concentrations, irrespective of the applied screening parameters [Fig. 4(a)]. It is noteworthy that the SFE first slightly drops and then rises above 5 at.% W addition with the screening parameter of 0.9. The reference data from the work of Tian *et al.*, calculated using the same method [28] with the screening parameter of 0.6, show a very weak decrease in the W content range from 0 to 5 at.%. Clearly, the difference stems from how the CPA error is treated. When we use the same screening parameter of 0.6, the results are in line with Tian *et al.* Accordingly, the effect of the selected screening parameter for Co-W alloy is significant, and previous work also verified this [4]. The difference between the two screening parameters amounts to about 12 mJ/m^2 for dilute Co-W alloys, which can be interpreted as the uncertainty of the absolute SFE values, while the concentration trend and the physical conclusions remain unchanged.

Upon W addition up to 5 at.%, the SFE is much lower than the value of pure Co at the same volume. We decouple the total SFE of $\text{Co}_{100-x}\text{W}_x$ into volume and chemical terms as

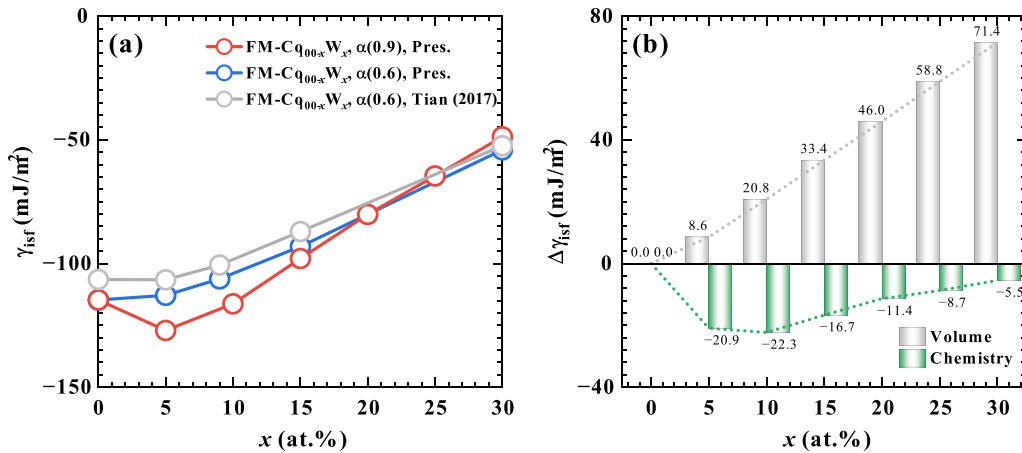


FIG. 4. (a) SFE of FM $\text{Co}_{100-x}\text{W}_x$ as a function of concentration, compared to the theoretical data from the literature [28]. (b) Decoupled effect of volume and chemical contributions on SFE shown relative to pure Co.

discussed previously. The SFEs consist of two contributions: the volumetric and chemical parts. The volumetric contribution is defined as the SFE difference in pure Co corresponding to volumes at different W compositions. The chemical contribution is defined as the difference between volumetric and total SFEs. Accordingly, the relative values of the volumetric and chemical effects for the $\text{Co}_{100-x}\text{W}_x$ system are given relative to the value of pure Co at equilibrium volume, plotted as a function of W concentration in Fig. 4(b). One can see that the volumetric effect dominates the variation of SFE, especially at larger W contents. However, the chemical effect from the bonding of W and Co atoms has a greater effect on SFE than the volumetric effect in the region up to a level of 10 at.% W, and one can see that the addition of W causes a decrease in total SFE at approx. 5 at.% W. The volumetric term grows almost linearly with W content, whereas the chemical term is strong in the dilute limit and weakens above 10 at.%. This yields a crossover of the minimum based on these two contributions of opposite signs. In summary, the volumetric effect is predicted to increase the SFE of the onCo-W system. However, the chemical effect is still significant at small W levels and is responsible for the local minimum in SFE versus W content. Since W addition to Co also affects magnetism, one expects a direct magnetic effect SFE. Namely, since hypothetical nonmagnetic Co has the fcc lattice, gradually removing magnetism by W doping should have a positive effect on the SFE. In the present analysis, this effect is part of the chemical effect shown in Fig. 4(b), and it is likely to be responsible for the decrease (in absolute value) of the chemical effect at W contents above approx. 10 at.%. Previous experimental works observed that heavy elements (such as W) could segregate to the stacking fault layer in Co-based alloys [6,66,67]. We calculate the effective chemical potential of W in bulk and at the stacking fault layer for $\text{Co}_{100-x}\text{W}_x$. The tests can be found in SM Fig. S2 [47]. The results show that W prefers to remain at the stacking fault layer until the addition of W exceeds approximately 10 at.%. It is concluded that W stabilizes the hcp structure at low concentrations, but above 10 at.% W, the hcp structure becomes less stable.

In addition, it is known that there is a big difference in radii between Co and W atoms. We thus consider the influence of segregation on SFE and calculate the SFE of pure Co with an accumulation of W in the stacking fault layer to simulate the segregation of W. We notice that here the bulk is pure Co (or more precisely, a dilute Co-W alloy) and thus, according to the previous results, there is a driving force for W to move to the stacking fault layer. We do not establish the equilibrium concentration profile; instead, we consider how the SFE is affected when W segregates to the stacking fault. We should emphasize that this segregation-induced change of the SFE is estimated under static conditions without accounting for any entropy (like the configurational entropy) effects. The results are tabulated in Table S2 [47] (refer to segregation). Here we consider an additional 5–30 at.% W in the stacking fault layer for pure Co. According to our results, the stable fault energies, for γ_{isf} and γ_{tw} , slightly decrease with increasing W concentration, indicating that the segregation of W reduces the fault energy, which is known as Suzuki segregation. The unstable fault energies (γ_{usf} and γ_{utw}) show the opposite trend, implying that the addition of W to the stacking fault layer in-

creases the energy barrier. For comparison, in VASP calculation for segregation, we use a stacking fault configuration with 25 at.% W (one W occupies the SF layer) added to the stacking fault layer in VASP. We fix the lattice parameter to 3.530 Å and allowed for full relaxation. The so obtained VASP results for γ_{isf} , γ_{usf} , γ_{utw} , and γ_{tw} are −133.5, 334.2, 261.0, and −122.0 mJ/m², respectively. The VASP results agree well with the EMTO results (Refer to Segregation, the results of Co-25W in Table S1) [47], showing the same segregation tendencies.

Further investigations examine how elemental segregation at different positions, i.e., at varying distances from the stacking fault plane, affects the SFE of Co using VASP. Specifically, the cases considered include segregation directly at the stacking fault layer (SF-0, shown in Fig. 1), at the first neighboring layer (SF-1), and at the second neighboring layer (SF-2). For the SF-1 configuration, the VASP-calculated γ_{isf} , γ_{usf} , γ_{utw} , and γ_{tw} values are −124, 264, 207, and −113 mJ/m², respectively. For the SF-2 configuration, the corresponding values are −110, 255, 167, and −142 mJ/m². Averaging the results over the three segregation positions for γ_{isf} , γ_{usf} , γ_{utw} , and γ_{tw} yields −123, 284, 212, and −126 mJ/m². These results indicate that the closer W segregates to the fault layer, the stronger its influence on the SFE. Additionally, the values obtained for the SF-2 configuration closely match those of pure Co, suggesting that segregation effects in the second neighboring layer are minimal and can be reasonably neglected. At this point, we should notice that the above segregation study corresponds to a specific W level near the stacking fault layer. We should admit that the segregation can show a strong bulk concentration dependence, which is not considered here.

Figure 5 presents the SFE variation with increasing Al content for the $\text{Co}_{100-x}\text{Al}_x$ system. All the data can also be found in Table S3 [47]. The FM SFE slightly increases in the range from 0 to 10 at.% Al addition and subsequently decreases as the Al content increases further [Fig. 5(a)]. The addition of Al shows the opposite tendency compared to W addition. Also the influence of Al content on SFE of the $\text{Co}_{100-x}\text{Al}_x$ system combines the effects of volume and chemistry change. These two effects are decoupled in the same manner as described above for W and plotted relative to that of pure Co as a function of Al concentration in Fig. 5(b). The volumetric effect on SFE increases with increasing Al content, while the contribution to SFE from the chemical term first increases slightly up to approx. 5 at.%, but subsequently decreases with the further addition of Al. The chemical effect on the SFE is pronounced especially at high Al contents. With the segregation of Al to the fault layer, the SFE calculated by using the EMTO method slightly decreases with increasing Al, indicating that the addition of Al reduces the SFE and energy barrier (Table S2 [47]).

Subsequently, we investigate the variation of SFE for the FM $\text{Co}_{100-x}\text{Ni}_x$ system as a function of Ni content; all the data can be found in Table S4 [47]. Several experimental and theoretical data for comparison are available in this system, which makes it a valuable resource for researchers (Fig. 6). One can see that the SFE increases with increasing Ni content [Fig. 6(a)]. A similar decomposition for $\text{Co}_{100-x}\text{Ni}_x$ is shown in Fig. 6(c). The volumetric contribution is small and negative, since Ni only slightly reduces the lattice constant [as shown in Fig. 2(d)]. The chemical contribution is positive and

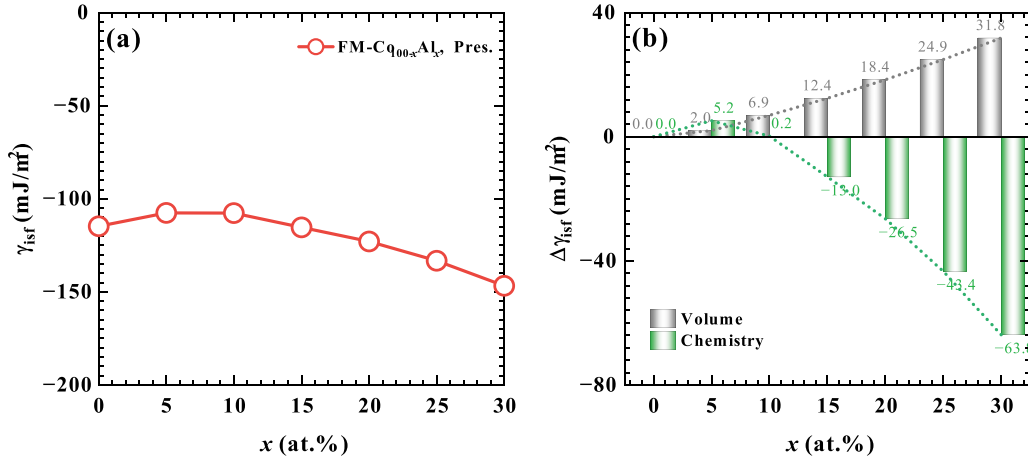


FIG. 5. (a) SFE of FM $\text{Co}_{100-x}\text{Al}_x$ as a function of concentration. (b) The effect of volume and chemical concentration on SFE plotted relative to pure Co.

dominates the whole concentration range. Thus the two terms cannot compete with each other, and no extremum forms, opposite to the $\text{Co}_{100-x}\text{W}_x$ case. In comparison with theoretical data from the literature [28,32] using the same EMT0 method with a screening parameter of 0.6, a good agreement with the present work is found, implying that there is no obvious influence on SFEs stemming from the screening parameter for

the $\text{Co}_{100-x}\text{Ni}_x$ system. Chandran *et al.* obtained an SFE value of -52 mJ/m^2 for $\text{Co}_{78}\text{Ni}_{22}$ using VASP in combination with the axial interaction model (AIM) approach [68]. It is close to the current calculated value shown in Fig. 6. Experimentally, the phase transformation in pure Co from α (fcc) to ε (hcp) takes place around 700 K on cooling [75]. Since 30 at.% Ni addition decreases the transition temperature to

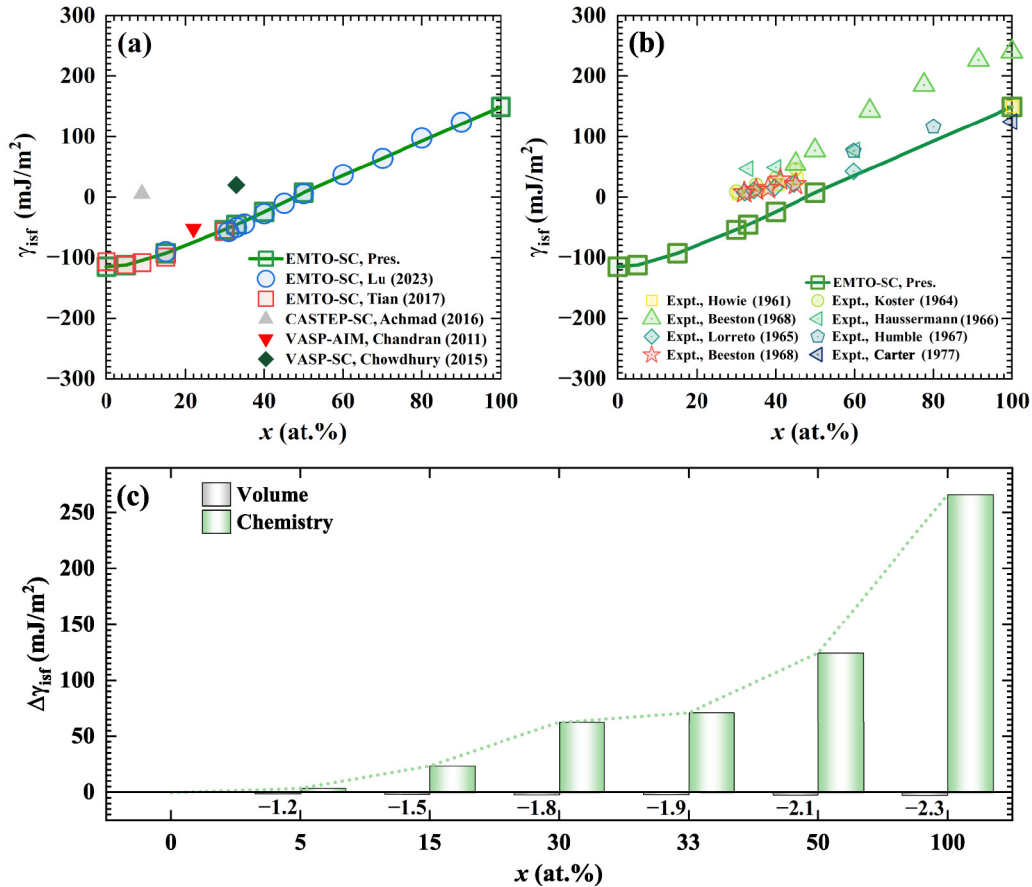


FIG. 6. SFE of FM $\text{Co}_{100-x}\text{Ni}_x$ as a function of concentration, compared with (a) theoretical [28,32,53,68,69] and (b) experimental data [64,70–74] from literature. (c) Decomposition of the SFE variation into volume and chemical contributions relative to pure Co.

300 K, one can expect the value of SFE at 0 K to be still negative due to the stability of the hcp phase. A positive value of 20 mJ/m² for Co₆₇Ni₃₃ was obtained using VASP with the supercell method [69]. We do not know the reasons for the discrepancy due to the missing details for the DFT calculation in Ref. [69].

When we compare the current results for Co_{100-x}Ni_x to the experimental data [64,70–74], we notice that the predicted SFE results show the same trend as the experimental data and are close to them. However, the experimentally determined SFE is always positive, resulting from the experimental measurement method for SFE based on the partial dislocation separation [32]. In comparison, theoretical calculations are in terms of the Gibbs free energy difference between the fcc and hcp phases but do not take into account the influence of the resistance to the movement of the partial dislocations (lattice friction) generating the stacking fault. Thus there should be a discrepancy coming from lattice friction between the experimental data and the DFT results, especially for metastable alloys with negative SFE. One can assume that the balance of two forces exists for one partial dislocation: the repulsive force and the attractive force. The direction of the lattice friction is opposite to that of the repulsive force for metastable cases, thus, the experimental value ($\gamma_{\text{isf}}^{\text{exp.}}$) should be the sum of the contributions of the repulsive force, the attractive force, and lattice friction. Namely, it is the sum of the theoretical value ($\gamma_{\text{isf}}^{\text{theo.}}$) and the excess value ($\gamma_{\text{isf}}^{\text{exc.}}$) using a well-documented relationship between the experimental and theoretical results [35,76]. They can be in good agreement with each other when the excess terms are included [76,77]. It should be noted that the stacking fault energies discussed in the preceding sections are intrinsic values directly obtained from first-principles calculations. To facilitate comparison with experimental measurements, which are influenced by deformation mechanics and grain-size effects, a semi-empirical relationship [Eq. (3)] is employed as suggested by Werner [76]. This expression can account for the difference between the theoretical intrinsic stacking fault energy and the experimentally measured effective stacking fault energy by considering the dislocation nucleation term. It is not introduced as an ad hoc correction to reconcile the theoretical and experimental values. Taking Co₆₇Ni₃₃ as an example, one can calculate the corrected value of SFE using the following equation:

$$\gamma_{\text{isf}}^{\text{theo.}} = \gamma_{\text{isf}}^{\text{exp.}} - b_p \left(\tau_{0,\text{twin}} + \frac{K_{\text{twin}}^{\text{HP}}}{\sqrt{D}} \right), \quad (3)$$

where $\tau_{0,\text{twin}}$ is the critical twinning resolved shear stress, $K_{\text{twin}}^{\text{HP}}$ is the Hall-Petch slope of critical twinning resolved shear stress, and D is the grain size. The $\tau_{0,\text{twin}}$ of Co₆₇Ni₃₃ is 27 MPa and b_p is $a/\sqrt{6}$ ($a = 3.521\text{\AA}$) [69]. The reported experimental value of SFE is 11.2 [70] or 15.5 mJ/m² [64] for Co₆₇Ni₃₃. Considering the excess term and neglecting the Hall-Petch term for larger grain sizes, the corrected value becomes -27.6 mJ/m^2 (or -23.3 mJ/m^2), which is negative and close to the present theoretical value of -45 mJ/m^2 , indicating that the present DFT calculations reliably predict the SFE. The nearly constant shift between the experimental and present theoretical values in Fig. 6(b) we ascribe to the

above effect and to the explicit thermal effects beyond the thermal expansion effect, which are not included in the present work.

We next attempt to qualitatively understand the trends in the stacking fault energies (SFEs) of the Co-W, Co-Al, and Co-Ni systems. We first emphasize that the decomposition of the total SFE change into different contributions is somewhat ad hoc, as briefly discussed in Section 2.2. In particular, we separate the volumetric contribution because fcc Co exhibits a pronounced positive dependence of the SFE on volume (Fig. 3). Since both W and Al increase the equilibrium volume of Co, a significant volumetric contribution is expected in both systems, as indeed observed in Figs. 4 and 5. In contrast, Ni produces only a weak negative volume dependence, resulting in an almost negligible volumetric contribution to the SFE of CoNi (Fig. 6). In all three systems, the volumetric contribution is approximately linear with concentration and therefore cannot account for the pronounced nonlinear behavior of the SFE, particularly in Co-W and Co-Al. We therefore focus below on the remaining contribution, here defined as a chemical contribution, which includes both the explicit electronic and magnetic effects.

We first consider the magnetic contribution. In Fig. 7(b), we show the energy difference between the hcp and fcc structures of Co as a function of magnetic moment, with the volume fixed at the theoretical equilibrium volume of ferromagnetic fcc Co. Since the SFE is proportional to the energy difference between the hcp- and fcc-like local environments, the relative stability of these two structures provides a useful insight into how alloying may affect the SFE. The calculated structural energy difference exhibits a pronounced minimum in the vicinity of the equilibrium magnetic moment, indicating a strong sensitivity of the hcp-fcc energy difference to the magnetic state.

Both W and Al additions reduce the magnetization of Co [Fig. 7(c)]. Consequently, alloying drives the system away from the minimum in the magnetic energy difference and generally increases (decreases in absolute value) the energy difference between the hcp and fcc structures, thereby making the hcp structure less favorable relative to fcc. This magnetic contribution is substantially stronger in Co-W than in Co-Al because the magnetic moment of the Co atoms decreases more rapidly with W concentration. An additional feature arises at low W concentrations. Because the equilibrium magnetic moment of fcc Co is slightly larger than that of hcp Co (Ref. [75]), a small amount of W initially shifts the system toward the magnetic regime that favors hcp relative to fcc. With further W addition, the system moves beyond this regime, and the fcc structure becomes increasingly favored. This produces the weak local minimum in the magnetic contribution around 5 at.% W shown in Fig. 7(d). A similar minimum occurs in Co-Al, at approximately 10 at.% Al [Fig. 7(d)], although the magnitude of the magnetic contribution is generally smaller than in Co-W.

The remaining part of the chemical contribution, here referred to as the electronic contribution, can be rationalized in terms of the electronic density of states (DOS) of fcc and hcp Co (see Ref. [75]). The majority-spin states are essentially fully occupied in both structures, whereas the minority-spin DOS exhibits pronounced structure near the Fermi level. In

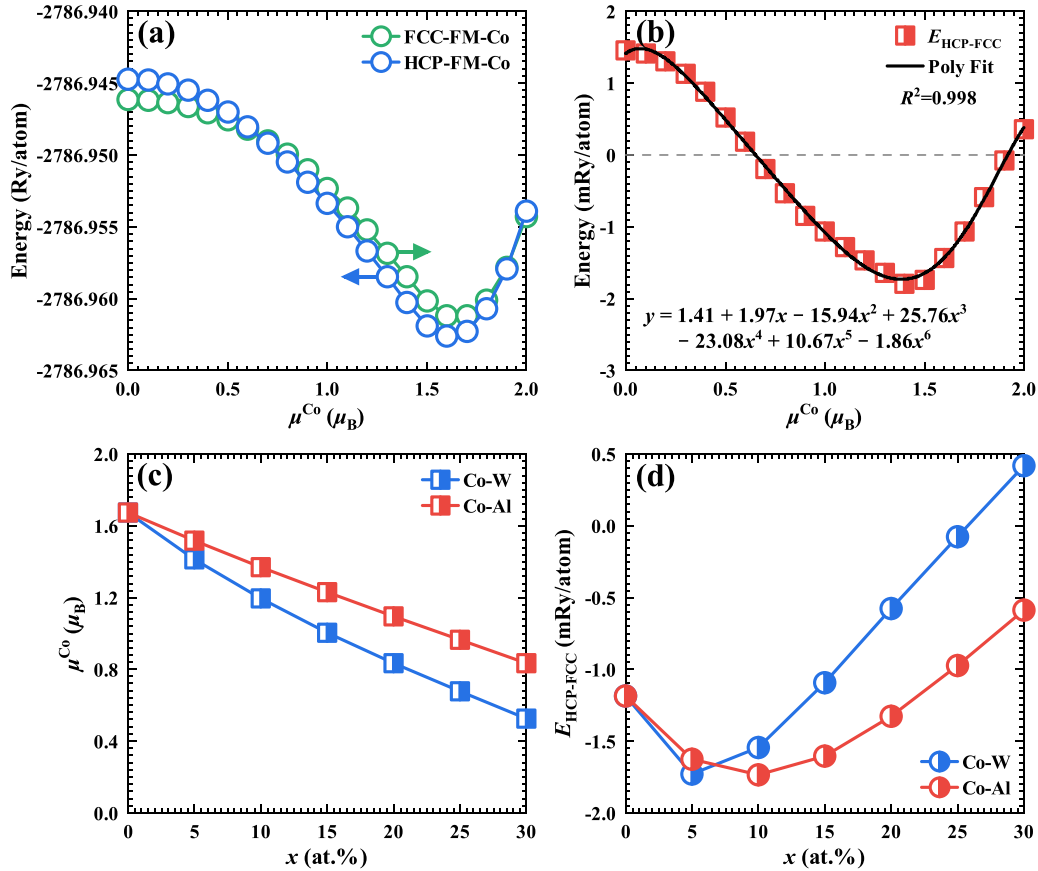


FIG. 7. Magnetic contribution to the hcp-fcc structural energy difference. (a) Total energies of ferromagnetic fcc and hcp Co calculated at the fcc equilibrium volume as a function of local magnetic moment. (b) Energy difference between the hcp and fcc structures of Co as a function of local magnetic moment. (c) Local magnetic moment of Co in CoW/CoAl alloy as a function of W/Al concentration. (d) Magnetic contribution to the structural energy difference in CoW/CoAl alloy as a function of W/Al concentration.

particular, the hcp phase has a local minimum in the minority-spin DOS close to the Fermi level, while the fcc phase exhibits a local maximum, with local minima immediately below and above the Fermi level. Addition of either W or Al reduces the number of valence electrons relative to Co and, within a rigid-band picture, shifts the Fermi level toward lower energies. The majority-spin channel is largely unaffected by this shift, whereas in the minority-spin channel the shift moves the Fermi level into a region that reduces the relative stability of hcp with respect to fcc. Thus, from this electronic contribution alone, both W and Al are expected to increase the SFE.

This effect is expected to be stronger for Al than for W because Al has no occupied d states, whereas W retains a substantial d-electron contribution (Co has 7d electrons). When combined with the magnetic contribution discussed above, these two effects lead to different concentration dependencies in Co-Al and Co-W. In the dilute Co-Al regime, the electronic/chemical contribution dominates over the magnetic and volumetric terms, resulting in an increase in SFE with Al concentration. In Co-W, on the other hand, the stronger magnetic contribution counteracts the electronic contribution and produces a weak decrease in SFE with increasing W concentration at low solute concentrations.

At large W and Al concentrations, the alloys become progressively less magnetic, and their behavior increasingly approaches that expected for nonmagnetic transition-metal

systems. According to the theory of crystal structures developed by Skriver [78], reducing the effective number of d electrons in nonmagnetic Co tends to stabilize the hcp structure relative to fcc. This effect is expected to be substantially stronger for Al than for W because Al more effectively reduces the effective d-electron count.

Consequently, at high solute concentrations, the electronic contribution becomes sufficiently large to dominate the volumetric and magnetic contributions in Co-Al, resulting in the observed decrease in SFE. In Co-W, in contrast, the electronic contribution is weaker because W retains a substantial d-electron contribution. The approximately linear and positive volumetric contribution, together with the remaining positive magnetic contribution, therefore becomes dominant at high W concentrations, leading to an overall increase in the SFE. Finally, it is worth noting that Ni addition increases the effective number of d electrons, shifting the Fermi level into a region of the DOS associated with greater fcc stability and thereby producing a positive electronic contribution to the SFE.

C. $\text{Co}_{81.7}\text{Al}_{18.3-x}\text{W}_x$ alloys

Reinforcing γ' precipitates with $\text{L}1_2$ structure are known to be particularly effective for high-temperature strengthening of superalloys. The $\text{Co}_3(\text{Al}, \text{W})$ γ' phase was first found in the

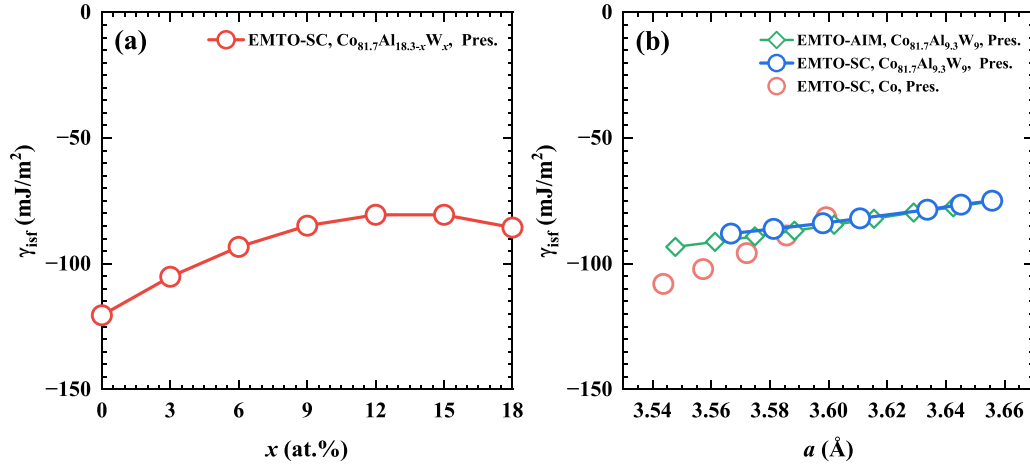


FIG. 8. SFE of Co-Al-W alloys (a) SFE for $\text{Co}_{81.7}\text{Al}_{18.3-x}\text{W}_x$ as a function of concentration and (b) for $\text{Co}_{81.7}\text{Al}_{9.3}\text{W}_9$ as a function of volume.

Co-Al-W system [1]. At elevated temperatures, the L1_2 precipitate will partly dissolve during service, causing a variation of Al and W concentrations in the γ matrix [2]. To determine how the SFE of a respective matrix phase changes with Al and W contents, the SFE of random FM $\text{Co}_{81.7}\text{Al}_{18.3-x}\text{W}_x$ ($0 \leq x \leq 18.3$) with fcc structure is calculated and plotted as a function of W content in Fig. 8(a). At $x = 0$, the SFE is -120 mJ/m^2 [see Fig. 8(a)]. When adding W to this alloy, the SFE first increases at the beginning and then decreases slightly as the W content increases beyond 12 at.%. It can be inferred that the hcp phase becomes less stable with W addition to the $\text{Co}_{81.7}\text{Al}_{18.3}$ alloy. It is noteworthy that W addition to pure Co (see Fig. 4) initially decreased the SFE. Therefore the positive slope of SFE at low W levels in Fig. 8(a) has to be due to a synergistic effect of Al and W.

According to the correlation between chemistry and SFE for $\text{Co}_{100-x}\text{W}_x$ and $\text{Co}_{100-x}\text{Al}_x$ systems, as mentioned in Sec. III B 2, the SFE is found to be nearly linearly dependent on volume, while it shows a non-linear behavior in terms of chemical composition. In particular, the chemical influence dominates the variation of the SFE at low concentrations of Al or W, and nonlinear concentration dependence was found in $\text{Co}_{81.7}\text{Al}_{18.3-x}\text{W}_x$ alloys. Eventually, it balances the synergistic effect of Al and W, and the critical content of W is ~ 12 at.%. In previous experimental work, Pyczak *et al.* studied the effect of varying W contents on the creep properties of ternary Co-Al-W alloys, the range of W being from 8 to 11 at.%, while the concentration of W in the γ matrix was up to 10 at.% [8]. Currently, additional elements are considered to fully or partially substitute W to lower the density and achieve better stability of the hardening γ' phase. At the same time, alloying also influences the partitioning coefficient of W between the γ matrix and L1_2 γ' precipitates.

Taking a closer look at the ternary Co-based alloy with the nominal composition of 9 at.% Al, 9 at.% W and Co balanced, the specific composition of the γ matrix is $\text{Co}_{81.7}\text{Al}_{9.3}\text{W}_9$ measured by TEM-EDX [8]. The calculated SFEs are plotted as a function of volume for $\text{Co}_{81.7}\text{Al}_{9.3}\text{W}_9$ [Fig. 8(b)]. One can see that the SFE increases steadily with increasing volume and that the supercell method and the first-order term of AIM show the same trend. The synergistic effect of Al and W increases

the SFE value relative to that of pure Co and stabilizes the fcc phase.

D. Temperature dependence of stacking fault energy

1. Pure Co

Figure 9(a) shows the SFE of Co in different magnetic states as a function of temperature. The FM SFE increases with increasing temperature, which means the fcc structure is stabilized with increasing temperature. Theory shows a similar trend as the available experimental data [64] and thermodynamic calculations of SFE with respect to temperature, and the results are fitted to the experimental SFE values [29,75]. However, the corresponding PM SFE shows an opposite trend with increasing temperature. Recall that we merely considered the thermal lattice expansion using the experimental lattice constant at the corresponding temperature. Ishida *et al.* attempted to estimate the stacking fault energy by a thermodynamic estimation in comparison with experimental data and verified the critical magnetic contribution on the SFE of magnetic metals, including Fe-, Co-, and Ni-based alloys [29]. In particular, they reported that the magnetic effect is important to explain the high SFE value in Co-based alloys and austenitic stainless steels, and one can see that their estimations resemble the trend of the available experimental data [Fig. 9(a)]. If we use the experimental data to extrapolate the SFE to 0 K, it should then be -50 mJ/m^2 upon considering the error [28], as shown by the star symbol in Fig. 9(a). Accordingly, it can be inferred that the value of SFE considering excess contributions should be between the present FM and PM SFE values.

When taking into account the magnetic contribution, the PM(Mag.) SFE decreases with increasing temperature and is slightly lower than that without the magnetic contribution (PM SFE). The weak dependence of PM SFE (or fcc-hcp energy difference) on volume expansion (temperature) was also observed when comparing the equations of state for PM fcc and PM hcp in Ref. [29]. Furthermore, one should consider the temperatures of phase transformation and magnetic transition as indicated by the dashed line in Fig. 9(a). It is known that the experimental phase transformation temperature is 700 K,

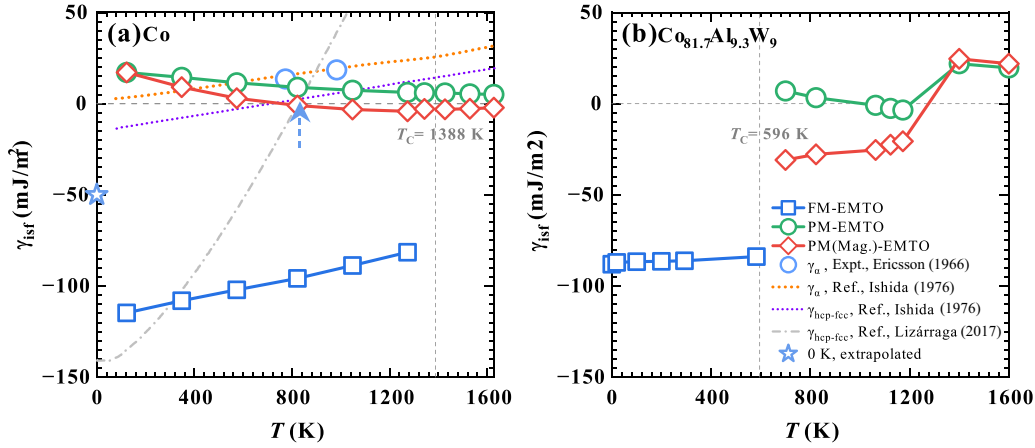


FIG. 9. SFE calculated as a function of temperature at different magnetic states (a) for Co and (b) for $\text{Co}_{81.7}\text{Al}_{9.3}\text{W}_9$. The lattice constant at each temperature is taken from experimental thermal expansion measurements [8,52]. The gray dash-dotted line in (a) shows $\gamma_{\text{hcp-fcc}}$ obtained by applying the first-order AIM to the free energies of Ref. [75], which crosses zero near 825 K (marked by the arrow). The open star symbol at 0 K marks the linear extrapolation of the experimental SFE data, about -50 mJ/m^2 [28]. Other theoretical calculations [29] and experimental data [64] are also included for comparison in (a). The magnetic contribution term is included for the PM state, denoted as PM (Mag.). All the numerical values are presented in Table S5 [47].

while the theoretical prediction is about 825 K [75]. From Fig. 9(a), we notice that as the temperature increases to 700 K, the FM SFE is still negative, while it should be positive because the fcc phase is more stable than the hcp phase. This discrepancy is likely due to the fact that important thermal effects are not included in the present calculations. These are vibrational and electronic excitations, electron-phonon interaction, quasi-harmonic, and longitudinal spin fluctuation contributions, as discussed in Ref. [75]. Therefore we extracted the free energy in Ref. [75] and adopted the first-order axial interaction model (AIM) method to calculate the SFE ($\gamma_{\text{hcp-fcc}}$), which includes all contributions at the FM state, and plotted it in Fig. 9(a), as the gray dash-dotted line shows. One can expect that the SFE should be 0 at 825 K, as shown by the blue arrow in Fig. 9(a). When temperatures increase further to 1388 K, the PM SFE should be positive as the fcc structure is more stable than the hcp structure, showing reasonable values for the temperature effect. Subsequently, the SFE should undergo a decrease as the temperature exceeds the magnetic transition temperature (1388 K [52]), as shown in the present calculated PM SFE and PM(Mag.) SFE [Fig. 9(a)]. However, this decrease cannot be as sharp as suggested in Fig. 9(a) since the magnetic transition is a second-order transition and magnetic softening occurs far below the Curie point.

Despite the fact that the magnetic contribution at high temperatures could become small, as the difference in magnetic moments and entropies decreases based on previous work [34], it does change the PM SFE from positive to slightly negative. The very small SFEs at the PM state are expected to have a significant effect on the activated deformation mechanism of Co and Co alloys, as discussed in the following sections.

2. $\text{Co}_{81.7}\text{Al}_{9.3}\text{W}_9$ alloy

For the Co-Al-W gamma matrix, the Curie temperature ($T_C = 596 \text{ K}$) is significantly reduced compared to that of pure Co, thus, the effect of magnetic transition on the SFE

becomes more relevant for studying the deformation behaviors at elevated temperatures. Figure 9(b) presents the SFE of $\text{Co}_{81.7}\text{Al}_{9.3}\text{W}_9$ as a function of temperature. At low temperatures, it shows the same trend as that of pure Co in both FM and PM states. When the temperature is above the Curie temperature, the PM SFE without considering the magnetic contribution remains positive and decreases with increasing temperature up to 1173 K, and then increases as the temperature further increases. In particular, the PM SFE becomes sizable and positive at higher temperatures. When the magnetic entropy contribution is included, the PM(Mag.) SFE continuously increases with increasing temperature, and the value changes from negative to positive around 1200 K. It is interesting to note that the trends in the case of PM and PM(Mag.) SFE with increasing temperature for $\text{Co}_{81.7}\text{Al}_{9.3}\text{W}_9$ alloys are different compared to the case in pure Co, which is ascribed to the variation in the magnetic moment of the Co atom, as shown in Figs. 10(b) and 10(d) and discussed in the following.

IV. DISCUSSION

The magnetic effect on SFE is important for predicting the plastic deformation mechanism of magnetic materials, as previous investigations in Co- [25,29,75], Ni- [79], and Fe-based [34,36] alloys show. Therefore we investigate the variation of magnetic moments with volume in fcc and hcp phases and with the distance to the SF layer, i.e., the magnetic moments of Co atoms located at different distances from the stacking fault layer. The magnetic moment of a Co atom in the stacking fault layer is designated as SF-0. The magnetic moment of one in the layer situated at the first neighbor of the stacking fault is referred to as SF-1, and that of one in the layer situated at the second neighbor of the stacking fault as SF-2, as shown in Fig. 1(b). These moments are compared to the magnetic moment of the corresponding perfect bulk, to understand the different trends of FM and PM SFE and the

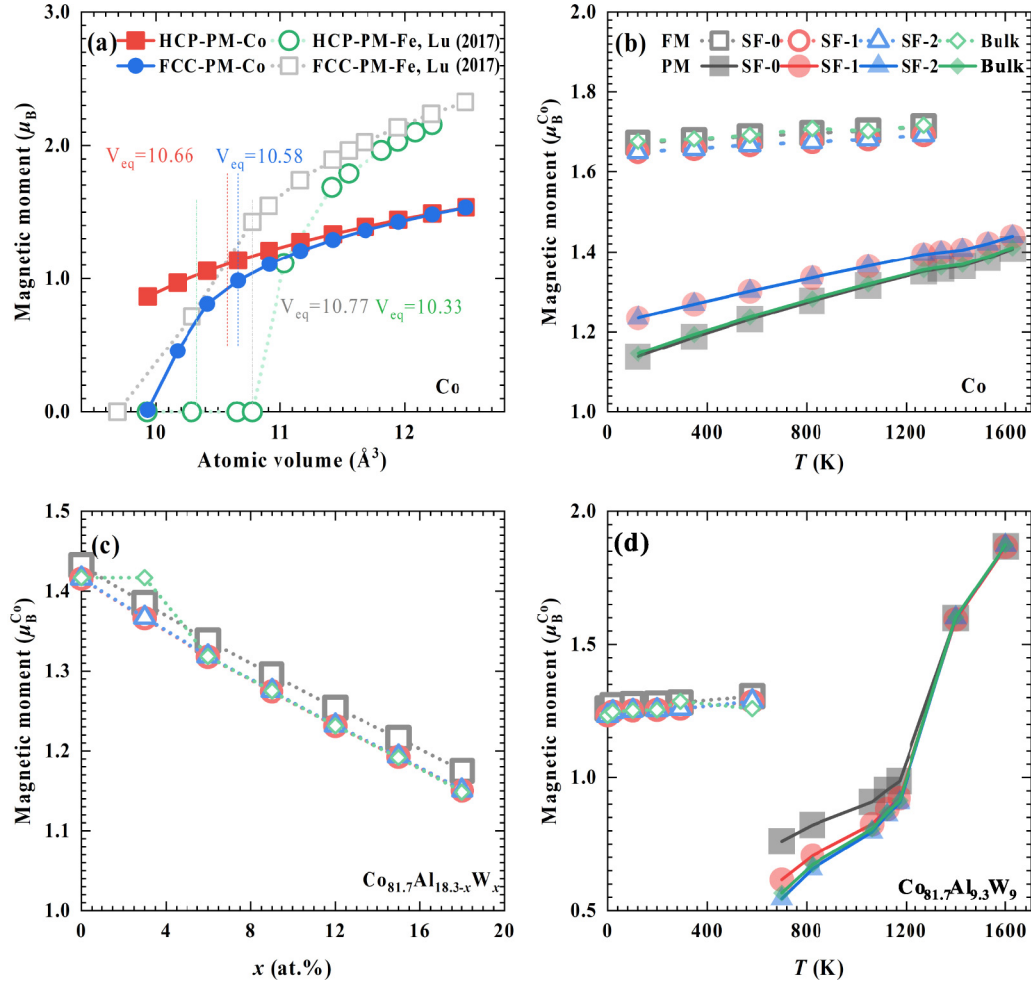


FIG. 10. Variation of magnetic moment of Co atom: (a) self-consistent local magnetic moment for pure PM Co and PM Fe [36] as a function of volume, (b) local magnetic moment in a supercell with a defect and perfect bulk in pure Co as a function of temperature, (c) local magnetic moment in a supercell with a defect and perfect bulk in $\text{Co}_{81.7}\text{Al}_{18.3-x}\text{W}_x$ as a function of concentration, and (d) local magnetic moment in a supercell with defect and perfect bulk in $\text{Co}_{81.7}\text{Al}_{9.3}\text{W}_9$ as a function of temperature. Note that the magnetic moments of the Co atom in (b)–(d) are extracted from those at the different distances to the stacking fault layer, namely, the magnetic moment of the stacking fault layer (SF-0), the layer situated at the first neighbor of the stacking fault layer (SF-1), and the layer situated at the second neighbor of the stacking fault layer (SF-2), and compared to the magnetic moment of the perfect bulk. The schematic is shown in Figs. 1(a)–1(c).

different magnetic contributions to SFE compared to previous results obtained for Fe [34].

A. Magnetic influence on stacking fault

Figure 10 illustrates the variation of the magnetic moment of Co atoms as a function of volume, temperature, and composition. Figure 10(a) shows the volume-dependent magnetic moments of PM hcp and fcc Co. We compare the Co moments with those of PM hcp and fcc Fe. Figure 10(b) presents the magnetic moments of FM and PM Co at different layer distances from the SF layer within the supercell, together with the corresponding values in the perfect bulk for pure Co. The magnetic moments of Co atoms at various layer distances to the SF layer in the supercell and those of the perfect bulk for $\text{Co}_{81.7}\text{Al}_{18.3-x}\text{W}_x$ series are shown in Fig. 10(c). Finally, Fig. 10(d) displays the magnetic moments of Co atoms at various layer distances to the SF layer and those of perfect bulk for the $\text{Co}_{81.7}\text{Al}_{9.3}\text{W}_9$ alloy [Fig. 10(d)].

The present calculated magnetic moment of FM Co is $1.68 \mu_B$ and is in excellent agreement with literature [63,80], while the magnetic moment of PM Co is $1.15 \mu_B$ at 0 K [Fig. 10(b)]. One can see that the magnetic moment of Co atoms increases with increasing volume (temperature) in Figs. 10(a) and 10(b). In Fig. 10(a), the local magnetic moments of fcc PM Co, after initially being zero, increase with increasing volume, while a finite magnetic moment is already present in the hcp structure prior to the fcc structure. The situation in PM Fe shows the opposite trend: the magnetic moment of fcc is activated before that of the hcp structure [36] (Fig. 10(a)). Consequently, the magnetic entropy contribution to SFE [Eq. (2)] in Co is negative, while in fcc Fe it is positive. Previous work has proved that the weakening of magnetism alone is not sufficient to destabilize the hcp phase at 700 K for Co [75], as proved by the slight increase in the magnetic moment of the FM Co atom in Fig. 10(b). It is known that the magnetic transition happens at 1388 K [52], while the structural transition occurs at 695 K [52] and accordingly,

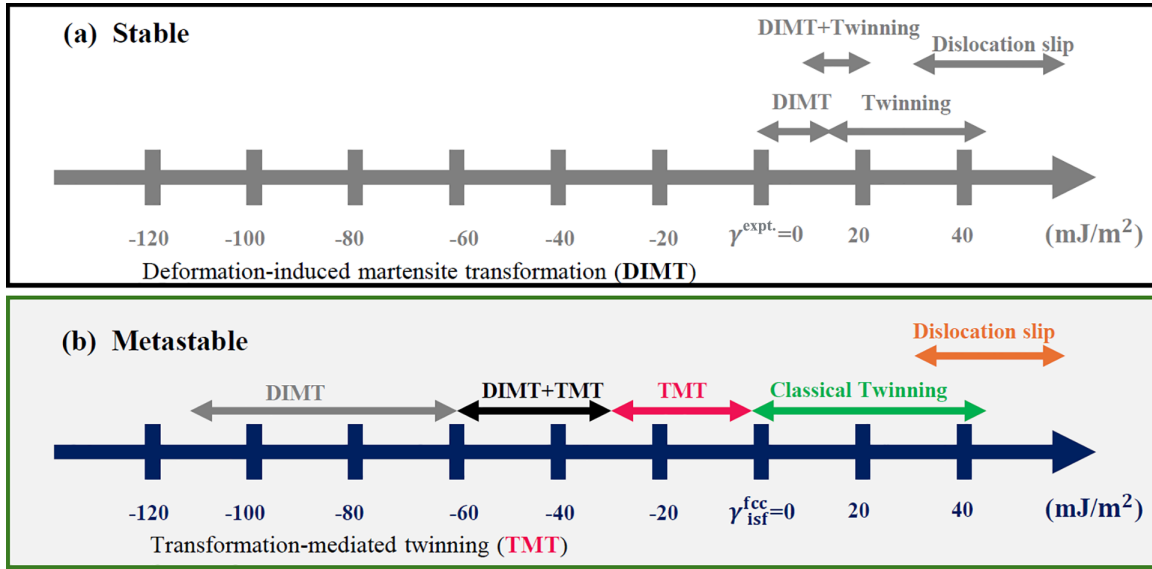


FIG. 11. Empirical relationship between SFE values and deformation modes for (a) stable alloys proposed experimentally [20], and (b) metastable alloys revised based on theoretical predictions [32].

it is anticipated that the determining factors influencing the structural transition in Co are more complex than the effect of magnetism alone. For Fe, the bcc-fcc structural transformation temperature is slightly higher than the Curie temperature. The situation of structural transition in Fe is clearly due to the loss of the magnetic order since in the magnetically disordered state the fcc phase is more stable than the bcc one [81].

To investigate the influence of W, the magnetic moments of the Co atom at different distances from the SF layer in the supercell are determined for the $\text{Co}_{81.7}\text{Al}_{18.3-x}\text{W}_x$ system and compared with these of the Co atom in perfect bulk at different W contents [Fig. 10(c)]. The magnetic moment of the Co atom in the stacking fault layer (SF-0) in the $\text{Co}_{81.7}\text{Al}_{18.3-x}\text{W}_x$ system decreases from $1.43 \mu_B$ to $1.18 \mu_B$ with increasing W content. The magnetic moment of the Co atom in perfect bulk (denoted as Bulk) decreases to $1.42 \mu_B$ due to the addition of Al and W, and further decreases with increasing W addition to $1.15 \mu_B$ [Figs. 10(b) and 10(c)]. Moreover, one can see that the magnetic moment of the Co atom located at the SF layer is larger than those in other layers in the $\text{Co}_{81.7}\text{Al}_{18.3-x}\text{W}_x$ system. The larger the distance between the layer of the Co atom in question and the SF, the closer the magnetic moment is to that of the perfect bulk, and the magnetic moment of a Co atom in the third layer is the same as that of a Co atom in the perfect bulk [Figs. 10(b) and 10(c)], indicating that the effect of magnetism on SFE can be neglected on the second-neighbor SF layer and the stacking fault configurations used in the present work are large enough to avoid the effect of periodicity.

For $\text{Co}_{81.7}\text{Al}_{9.3}\text{W}_9$ [Fig. 10(d)], the magnetic moment of the Co atom increases with increasing temperature, showing a similar trend to that in pure Co [Fig. 10(b)]. In particular, the magnetic moment of PM Co increases from $0.57 \mu_B$ to $1.87 \mu_B$ as the temperature increases. Therefore it can explain the similar trend of SFE in Fig. 9(b), when the magnetic contribution is included. It is therefore vital that the correct

magnetic state of the alloy is taken into account in *ab initio* calculations.

B. Deformation mechanism

Previous work unveiled an empirical relationship between the experimental positive SFE and the deformation mode for stable alloys [20], as shown in Fig. 11(a). However, due to the negative SFE values of metastable alloys, like Co [28], Co-Ni alloys [32], and CoCrNi alloys [35], this experimental relationship is not directly applicable to SFEs from *ab initio* calculations in metastable alloys. Therefore a revised version of the deformation mode map was proposed [32] [Fig. 11(b)] using theoretical calculations based on DFT, which, combined with the experimental investigation, could explain the individual deformation mechanisms with respect to the specific SFE value. It demonstrates the possibility to design desired mechanical properties by tuning the SFE value.

For pure Co, experimental work has deduced that the SFE of Co at 0 K should be negative [28,29,64], as already mentioned. The present calculated SFE value is negative and quite low (-114.7 mJ/m^2), implying continuous formation of the hcp phase, namely, martensitic transformation. The ongoing transformation with increasing strain also implies an increasing partial dislocation density. With continuous external stress, the SF will transform into an fcc twin to release the local stress, which is referred to as the transformation-mediated twinning (TMT) mechanism [32] in a metastable system (negative values of SFE). Specifically, the transformation from SF to fcc twin occurs when partial dislocations slip and thicken the HCP structure to six atomic layers. With increasing local strain and stress within the $\{111\}$ planes, the existing local HCP structure with six atomic layers transforms, starting from the next-nearest neighbor rather than the nearest neighbor. This sequence changes from “...ABCACACACABC...”, “...ABCACBACABCA...” to “...ABCACBACBCAB...” to decrease the free energy required to accommodate the inner

(lattice misfit) and external (applied stress) stresses during deformation.

This TMT mechanism explains why twinning takes place in pure Co and CoCrNi-based alloys at room temperature. Other theoretical [82,83] and experimental [84–86] works more or less showed a similar evolution of deformation modes. Moreover, alloys exhibiting the TMT mechanism demonstrate superior mechanical performance [32,35], as deformation twinning in fcc systems with negative stacking-fault energy is controlled not by conventional successive partial slip but by a transformation-mediated pathway in which a thermodynamically driven fcc $\rightarrow$ hcp transition is followed by an hcp $\rightarrow$ fcc twin reversion, producing a high density of twin boundaries through easier partial-dislocation activity and thereby enhancing both strength and ductility.

For Co-Ni-based alloys, experiments find that deformation twins form in the temperature range of $298\text{ K} \leq T \leq 400\text{ K}$ when the SFE values are in the range of $15\text{--}20\text{ mJ/m}^2$ with 30%–34% Ni [20,64,70] additions. There is even an extended range between $15\text{--}50\text{ mJ/m}^2$, depending on the exact compositions of alloys [20]. Ericsson *et al.* [64] and Rémy *et al.* [20] reported that a Ni content of 33 at.% decreases the phase transformation temperature from fcc to hcp of pure Co from 693 K to 173 K [64]. The formation of twins at room temperature in $\text{Co}_{67}\text{Ni}_{33}$ alloy was experimentally examined [20], and the twinning increases with increasing Ni concentration. Note that the present calculated theoretical SFE of $\text{Co}_{67}\text{Ni}_{33}$ is -45 mJ/m^2 , which is still negative and explains the occurrence of twinning in the alloy by the TMT mechanism. Importantly, this mechanism explains the coexistence of twinning and martensitic transformation as observed in experiments.

For $\text{Co}_{81.7}\text{Al}_{9.3}\text{W}_9$ SFE, one may expect similar deformation mechanisms as those in pure Co [32,87] and Co-Ni [20] alloys at elevated temperatures. The temperature dependence of SFE for the $\text{Co}_{81.7}\text{Al}_{9.3}\text{W}_9$ in Fig. 9(b) indicates that the TMT mechanism may also be activated at elevated temperatures above the Curie temperature. There is no experimental work available, but the criteria of twinnability (τ_a) proposed by Tadmor *et al.* [65] indicate the formation of twinning, since the τ_a of pure Co is 1.02 in the FM state, while 1.15 in the PM state (Table I), which are higher than that of $\text{Co}_{81.7}\text{Al}_{9.3}\text{W}_9$, being 1.09 in the FM state. The τ_a of $\text{Co}_{81.7}\text{Al}_{9.3}\text{W}_9$ is higher than that of pure Co, which is 1.09 in FM state at 0 K. In addition, the dimensionless parameter γ_d established by Jo *et al.* [22] implies that full slip with twinning will occur in stable alloys for values of $0 \sim 2$. However, for metastable Co and Co-based alloys with fcc structure, this parameter does not work anymore. Nevertheless, taking the value ($\gamma_d = -0.3$ in the FM state) of pure Co as a benchmark, twinning should be found in the $\text{Co}_{81.7}\text{Al}_{9.3}\text{W}_9$ which exhibits $\gamma_d = -0.2$ in the FM state.

While the γ matrix of Co-based alloys frequently has a quite complex composition, the main constituents of the matrix in a typical Co-based superalloy are Co, Ni and Cr. Accordingly, to resemble the situation in a typical Co-based superalloy matrix, the SFE of CoNiCr alloys is calculated. Experimentally, twins of 1 nm thickness with six atomic layers are observed in a CoCrNi-based superalloy, at a plastic strain of 3.0%, which subsequently thicken as the plastic strain increased to 3.5% at room temperature [88]. Therefore, for

DFT calculations, the $\text{Co}_{60}\text{Ni}_{40-x}\text{Cr}_x$ system is adopted to investigate the influence of chemical composition on the SFE. The relevant results are presented in Table II. The calculated SFE of the CoNiCr system complies well with the available theoretical data [32,91]. Chromium decreases the SFE of the $\text{Co}_{60}\text{Ni}_{40-x}\text{Cr}_x$ system up to a Cr content of 15%, where the minimum SFE value of -67 mJ/m^2 is found. Theoretically, for such SFE values, twinning by the TMT mechanism should be observed, τ_a and γ_d , which is also validated by experimental observation.

A large amount of experimental data for comparison with theoretical predictions exists for CoCrNi medium-entropy alloys, which is well-documented [25,32,35,58,87,91]. The chemical composition of the complex γ matrix of Co-based superalloys is rather similar, thus justifying the correlation of deformation modes in the CoCrNi medium-entropy alloys and the complex γ matrix for further validation. Recently, Chu *et al.* [87] have observed the formation of twins with six atomic layers and the evolution of deformation twins using in-situ transmission electron microscopy (TEM) in a CoNiCr alloy. In addition, the temperature and chemical composition affect the formation of deformation twins. For instance, twinning can be observed at 483 K for large elongations (10%–20%), while dislocation cells form for small elongations, or occur at the beginning of the deformation at 388 K. If the temperature decreases to 298 K or 77 K with strains of 10%, martensite forms in the $\text{Co}_{40}\text{Cr}_{16}\text{Ni}_{44}$ alloy (corresponding to the T3 alloy in Ref. [20]). The present calculated SFE value for this alloy is -5 mJ/m^2 , which is in good agreement with the result in Ref. [32]. In contrast, in the $\text{Co}_{54}\text{Cr}_{16}\text{Ni}_{30}$ alloy (representing the T6 alloy in Ref. [20]) with a calculated SFE value of -48 mJ/m^2 , some twinning can be observed at 298 K for strains of more than 30%. As the temperature decreases to 77 K, twinning is observed for 10% elongation, and twin density increases with increasing strain.

Therefore not only the chemical composition and temperature but also the conditions of plastic deformation matters for the CoNiCr system. Such parameters as the strain level [87], loading direction, and crystal orientation [69] affect the formation of twins. That could be the reason why deformation twins are not observed experimentally in the $\text{Co}_{60}\text{Cr}_{25}\text{Ni}_{10}\text{W}_5$ alloy, whose SFE value is -40 mJ/m^2 in the PM state in the present calculation, showing good agreement with the estimated value of -53 mJ/m^2 [90] by using the Olson-Cohen model.

For the more complex $\text{Co}_{35.4}\text{Ni}_{35.5}\text{Cr}_{22.9}\text{Mo}_{6.2}$ (known as MP35N alloy) [21], which exhibits good ductility and strengthens rapidly during cold working, twinning is found in the deformed matrix. For $\text{Co}_{34}\text{Ni}_{31}\text{Cr}_{24}\text{Mo}_6\text{Fe}_2\text{Nb}_1\text{Ti}_1\text{Mn}_1$ (commercial alloy SPRON510) [31], which is an fcc-type Co-Ni-based superalloy from room temperature to high temperature, one can see that the calculated SFEs increase with temperature but remain negative. Similar trends can be observed in both cases. Meanwhile, the calculated SFEs in the present work are within the SFE range of the TMT mechanism, and the values of τ_a and γ_d also indicate the twinnability, as shown in Table II.

The negative values can also explain the fine deformation twins appearing at elevated temperatures in experiments. This happens at high temperatures where dynamic recrystallization

TABLE II. The theoretically calculated SFEs for CoCrNi-base alloys. The available experimental and theoretical data are also included. All the numerical values can be found in Table S6 [47]. The composition of MP35N is $\text{Co}_{35.4}\text{Ni}_{35.5}\text{Cr}_{22.9}\text{Mo}_{6.2}$ [21]. The composition of commercial alloy SPRON510 is $\text{Co}_{34}\text{Ni}_{31}\text{Cr}_{24}\text{Mo}_6\text{Fe}_2\text{Nb}_1\text{Ti}_1\text{Mn}_1$ [31]. γ_d denotes the deformation parameter introduced by Jo *et al.* [22], while τ_a represents the twinnability in fcc structure, as defined in Ref. [65]. σ_{critical} corresponds to the critical twinning stress predicted by the analytical framework proposed by Kibey *et al.* [89].

Alloys (at.%)	Magnetic state	T (K)	a (Å)	γ_{usf} (mJ/m ²)	γ_{isf} (mJ/m ²)	γ_{utw} (mJ/m ²)	γ_{tw} (mJ/m ²)	γ_d	τ_a	σ_{critical} (MPa)
CoCrNi	PM	0	3.523	340.6	-20.5	329.8	-10.3	-0.06	1.13	315.0
	PM		3.526	338.4	-20.3	327.6	-10.2	-0.06	1.13	312.8
	PM		3.567	306.2	-17.1	297.0	-7.7	-0.05	1.13	284.4
$\text{Co}_{32.3}\text{Cr}_{36.3}\text{Ni}_{31.4}$	PM	0	3.526	331.8	-26.1	317.2	-16.7	-0.07	1.12	274.9
$\text{Co}_{37.5}\text{Cr}_{25}\text{Ni}_{37.5}$	PM		3.561	315.1	4.1	318.1	13.2	0.01	1.14	391.7
$\text{Co}_{40}\text{Cr}_{16}\text{Ni}_{44}$	FM		3.551	324.6	-5.2	324.5	8.7	-0.02	1.14	375.1
$\text{Co}_{54}\text{Cr}_{16}\text{Ni}_{30}$	FM		3.548	325.3	-48.9	301.7	-29.0	-0.13	1.12	186.5
$\text{Co}_{60}\text{Cr}_{10}\text{Ni}_{30}$	FM	0	3.526	334.5	-24.1	323.6	-2.1	-0.07	1.13	302.7
$\text{Co}_{60}\text{Cr}_{15}\text{Ni}_{25}$	FM	0	3.530	339.1	-32.2	325.5	-9.0	-0.09	1.13	282.1
$\text{Co}_{60}\text{Cr}_{10}\text{Ni}_{30}$	FM	0	3.531	342.0	-50.0	318.8	-26.6	-0.13	1.12	208.0
$\text{Co}_{60}\text{Cr}_{15}\text{Ni}_{25}$	FM	0	3.528	340.6	-67.8	307.4	-44.7	-0.17	1.11	126.5
$\text{Co}_{60}\text{Cr}_{25}\text{Ni}_{10}\text{W}_5$	FM	0	3.550	341.7	-87.9	293.4	-76.0	-0.20	1.09	14.4
	PM	300	3.589	347.2	-40.9	325.8	-27.5	-0.11	1.12	232.0
$\text{Co}_{60}\text{Al}_5\text{Ni}_{35}$			3.589 ^a		-53.4 ^a					
	FM	0	3.535	304.0	-20.8	297.6	-3.6	-0.06	1.13	296.9
	FM	0	3.540	304.8	-38.1	288.4	-21.2	-0.11	1.12	217.7
$\text{Co}_{60}\text{Al}_5\text{Ni}_{25}\text{W}_{10}$	FM	0	3.588	335.6	-18.9	327.2	-7.6	-0.05	1.13	319.7
$\text{Co}_{60}\text{Cr}_5\text{Al}_5\text{Ni}_{25}\text{W}_5$	FM	0	3.564	319.5	-34.9	303.5	-20.6	-0.10	1.12	240.0
MP35N [21]	FM	0	3.561	326.9	-21.2	314.5	-12.4	-0.06	1.12	285.7
	PM	300	3.572	328.8	-8.5	324.1	-0.6	-0.03	1.13	346.6
	PM	1000	3.600	302.1	-7.1	297.9	0.1	-0.02	1.13	317.8
	PM	1200	3.608	295.9	-6.7	291.9	0.2	-0.02	1.13	311.3
SPRON510 [31]	FM	0	3.574	308.1	-26.5	292.6	-19.9	-0.08	1.12	238.3
	PM	300	3.586	309.2	-18.1	299.0	-11.5	-0.06	1.13	279.4
	PM	1000	3.613	286.9	-15.8	277.9	-9.7	-0.05	1.13	261.2
	PM	1200	3.621	280.7	-15.4	272.0	-9.2	-0.05	1.13	255.5
	PM	300	3.586	309.2	-18.1	299.0	-11.5	-0.06	1.13	279.4
	PM	1000	3.613	286.9	-15.8	277.9	-9.7	-0.05	1.13	261.2
	PM	1200	3.621	280.7	-15.4	272.0	-9.2	-0.05	1.13	255.5

^aReference [90] calculated using the Olson-Cohen model.

(DRX) is usually dominant. Our *ab initio* calculations yield negative intrinsic stacking-fault energies for the Co-rich γ phase in the SPRON510 alloy, indicating that the fcc γ matrix is thermodynamically metastable with respect to ϵ -hcp. At elevated temperatures, leading partial dislocations glide on the $\{111\}$ planes if sufficient external stress is applied, and thereby generates stacking faults, namely ϵ -like lamellae in the γ channels. According to the transformation-mediated twinning (TMT) mechanism [32], these deformation-induced ϵ lamellae can subsequently transform back to fcc with reversed stacking via basal slips, producing γ twins in a $\gamma/\gamma_{\text{tw}}/\epsilon$ lamellar structure. At the temperatures where twinning is observed, solute-drag and Suzuki segregation of W (for W levels less than 10 at.%, it prefers the SF layer, the effective chemical potential of W in $\text{Co}_{100-x}\text{W}_x$ solid solution proves it) and other alloying elements at stacking faults are expected to reduce the local SFE and maintain a large separation of Shockley partials, which suppresses cross-slip and dynamic recovery, as reported for Co-Ni superalloys by Chiba *et al.* [31]. Consistent with the high-temperature microtwinning observed in Co-Ni-Cr-containing superalloys [7], deformation twinning in Co-Ni-Cr thus acts as an alternative

stress-relief mechanism once dislocation-controlled plasticity becomes inefficient. In this framework, negative SFE in the γ phase does not suppress twinning; instead, it promotes a $\gamma \rightarrow \epsilon \rightarrow \gamma_{\text{tw}}$ transformation pathway that enables twin formation at elevated temperatures. Consequently, judicious modification of SFE values through compositional tuning enables the attainment of desired mechanical properties at elevated temperatures, exemplified by other complex Co-based alloys. These findings underscore the significant predictive capability of *ab initio* calculations and their instrumental role in facilitating physics-based materials design.

V. SUMMARY

We investigated the GSFEs for pure Co and Co-based alloys using *ab initio* calculations. The effects of temperature, chemical composition, and magnetic state on SFE are systematically discussed. The plastic deformation mechanism is analyzed based on previously proposed relationships between SFE value and deformation mode. The main conclusions are as follows.

(i) The calculated FM SFE of pure Co increases with increasing volume, which is in good agreement with available theoretical data. The FM SFEs in binary $\text{Co}_{100-x}\text{M}_x$ ($M = \text{W}$ and Al , respectively) systems show a nonlinear behavior of SFE in terms of chemical composition in $\text{Co}_{100-x}\text{W}_x$ and $\text{Co}_{100-x}\text{Al}_x$ alloys. Specifically, the SFE first decreases and then increases with increasing W content, while the SFE shows the opposite trend with the addition of Al. The direct chemical influence and not the effect of chemistry on the volume dominates the variation of SFE for $\text{Co}_{100-x}\text{W}_x$ alloys for small W contents and for the $\text{Co}_{100-x}\text{Al}_x$ alloys in the whole range of Al contents. The variation of SFE in a ternary $\text{Co}_{81.7}\text{Al}_{18.3-x}\text{W}_x$ ($0 \leq x \leq 18$) system shows synergistic chemical effects of W and Al. The segregation of W and Al at the SF plane decreases the stacking fault energy and increases the stability of the hcp phase, which agrees well with experimental findings.

(ii) The SFE of $\text{Co}_{100-x}\text{Ni}_x$ calculated in the present work shows the same trend of increasing SFE with increasing Ni content as the available theoretical data and is also quite close to the experimental measurement if the excess contribution is considered, indicating the soundness of the current calculations.

(iii) It is important to take into account the correct magnetic state for predicting the SFE using *ab initio* calculations. The value of FM SFE significantly differs from the PM SFE in the case of pure Co and ternary $\text{Co}_{81.7}\text{Al}_{9.3}\text{W}_9$. The PM SFE decreases with increasing temperature in the case of pure Co and ternary $\text{Co}_{81.7}\text{Al}_{9.3}\text{W}_9$ in a finite temperature range, which is inconsistent with the temperature effect on stabilizing the fcc phase. Accordingly, the correct magnetic state should be considered when investigating phase stability.

(iv) In the case of pure Co, the magnetic moment increases as the volume increases, and the magnetic moment of the fcc

phase is slightly larger than that of the hcp phase in FM Co, while the magnetization assumes non-zero values in the hcp phase before that takes place in the fcc phase in PM Co. In addition, the magnetic moment of a Co atom at the SF layer is slightly larger than that of the bulk. The magnetic moment of a Co atom approaches that of the bulk material with increasing distance from the SF layer.

(v) The predicted negative SFE explains the formation of twins at elevated temperatures for a series of complex Co-based superalloys, which is also found experimentally. Moreover, this work demonstrates the significant potential of *ab initio* calculations to predict SFEs in Co-based superalloy matrix phases and, by this, gives valuable trends to tune the deformation mechanisms in those advanced materials.

ACKNOWLEDGMENTS

L.V. acknowledges the Swedish Foundation for Strategic Research (Grant No. SM23-0041), the Wallenberg Initiative Materials Science for Sustainability (WISE) funded by the Knut and Alice Wallenberg Foundation (KAW), the Formas—a Swedish Research Council for Sustainable Development (2023-00543), and the Swedish Foundation for International Cooperation in Research and Higher Education. S.L. and A.L. acknowledge the support from the European Union Project “Integrated Computational-Experimental material Engineering of Thermal Spray coatings” (GA No. “101092211, Project acronym: “CoBRAIN”). Computational resources were provided by the Helmholtz-Zentrum Hereon in Geesthacht.

DATA AVAILABILITY

The data are available upon reasonable request from the authors.

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