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ORIGINAL REPORT



# Plastic deformation transition in FeCrCoNiAl<sub>x</sub> high-entropy alloys

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## ABSTRACT

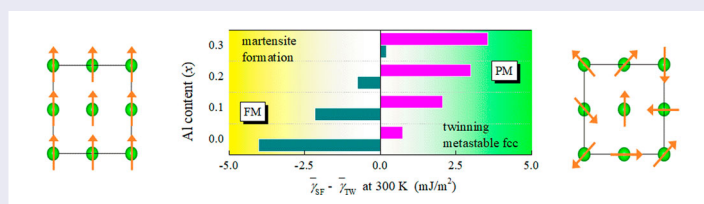
The competition between plastic deformation mechanisms in FeCrCoNiAl<sub>x</sub> high-entropy alloys is explored as a function of temperature by first-principle theory. Investigating the generalized stacking fault energy, we identify a strong interplay between the magnetic and chemical effects. At cryogenic conditions (ferromagnetic state), full-slip is accompanied by martensitic transformation, whereas increasing temperature towards room-temperature (paramagnetic state) changes the deformation mechanism to full-slip plus twinning. Alloying with Al reduces the susceptibility for stacking fault formation in the ferromagnetic state and promotes twinning in the paramagnetic state. The present advance in magneto-plasticity reveals new opportunities for tailoring the mechanical response in high-entropy alloys.

## ARTICLE HISTORY

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## KEYWORDS

High-entropy alloys; generalized stacking fault energy; TWIP/TRIP effects; ab initio calculations



## IMPACT STATEMENT

Magnetic state critically affects the  $\gamma$ -surface of FeCrCoNiAl<sub>x</sub> and is responsible for the emergence of the exceptional metastable twinning phenomena at room temperature.

The development of alloys with enhanced strength and ductility represents a continuous challenge in materials design. Over the past years, high-entropy alloys (HEAs) have generated considerable excitement for their unique combinations of mechanical properties [1–3]. For example, the equiatomic FeCrCoNiMn with single face-centered cubic (fcc) solid solution phase displays fracture toughness values at crack initiation well above 200 MPa m<sup>1/2</sup> associated with increasing tensile strengths from 730 to 1280 MPa as the temperature is lowered from 300 to 77 K [4]. Experimental observations indicated that the key to the unusual temperature-dependent strength and ductility is the presence of twinning as the dominant deformation

mechanism at cryogenic conditions [4]. More recently, the Fe<sub>80-x</sub>Mn<sub>x</sub>Co<sub>10</sub>Cr<sub>10</sub> alloys with a decrease of Mn content produce a partial martensitic transformation of the fcc phase to the hexagonal close-packed (hcp) phase at room temperature, i.e. the so-called transformation-induced plasticity (TRIP) assisted dual-phase HEAs, accompanied by a mechanical response similar to that of FeCrCoNiMn [5]. Since the deformation mode transition plays an important part in tuning the strength-ductility trade-off in such alloys, a theoretical understanding is indispensable for optimizing high-performance HEAs.

Generalized stacking fault energy ( $\gamma$ -surface), which represents the energy dependency of the rigidly sheared crystal within the fcc {111} plane along the  $\langle 11\bar{2} \rangle$

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direction, provides fundamental information in describing the deformation mechanism of the fcc metals [6]. The intrinsic stacking fault energy  $\gamma_{\text{isf}}$  is the excess energy associated with the stacking fault, and the unstable stacking fault energy  $\gamma_{\text{usf}}$  and the unstable twinning fault energy  $\gamma_{\text{utf}}$  determine the energy barrier to produce a stable stacking fault or a twin fault, respectively, within the pristine lattice. Various models based on  $\gamma$ -surface have been proposed to explore how planar faults multiply and interact [7–9]. So far, investigations of  $\gamma$ -surface for HEAs have been very limited, which can be attributed to the complexity of the problem related to the chemical and magnetic disorders. Using first-principle methods, here we reveal the temperature and composition-dependent  $\gamma$ -surfaces of the  $\text{FeCrCoNiAl}_x$  ( $0 \leq x \leq 0.3$ ) HEAs, which have been noted for their excellent combinations of strength and ductility [10–15]. We provide a detailed analysis of the chemical and magnetic contributions, explain the observed mechanical behavior, and predict the plasticity mechanisms at cryogenic and strain conditions. The considered HEAs were reported to possess a homogenous fcc structure [16–20]. In the present investigation, we focus on random solid solution state and neglect any possible local chemical ordering (LCO) effects discussed, e.g. in the case of CrCoNi medium-entropy alloys [21]. We expect that the LCO plays important role only for the initial stage of the deformation process and a substantial dislocation activity destroys the LCO produced by special heat treatments.

The present calculations are performed using the exact muffin-tin orbitals (EMTO) method [22], in combination with the coherent potential approximation (CPA) [23]. The one-electron Kohn–Sham equations are solved within the scalar-relativistic approximation and the soft-core scheme. The exchange–correlation effects are treated within the generalized gradient approximation [24]. The paramagnetic state is simulated by the disordered local moments (DLM) model [25]. Supercells consisting of nine fcc {111} layers with and without planar fault are applied, in which the chemical and magnetic (for the paramagnetic state) randomness is realized through the effective medium and single-site approximation as formulated within the CPA. Accordingly, all nine layers are occupied randomly by the alloy components and they are totally equivalent for the un-sheared case. The temperature-dependent lattice parameters are derived from room-temperature experimental value taking into account the linear thermal expansion coefficients [16,26]. The present approach has been applied previously to reveal various parameters and mechanisms for HEAs, and the reported results are in reasonable agreement with other theoretical results, as well as with the observations [27–35].

Figure 1(a) shows the  $\gamma$ -surface of the paramagnetic FeCrCoNi at room temperature. The first and second maxima are the unstable stacking fault energy  $\gamma_{\text{usf}}$  ( $\sim 290.5 \text{ mJ/m}^2$ ) and the unstable twinning fault energy  $\gamma_{\text{utf}}$  ( $\sim 289.5 \text{ mJ/m}^2$ ), respectively, and the first minima represent the intrinsic stacking fault energy  $\gamma_{\text{isf}}$  ( $\sim -0.3 \text{ mJ/m}^2$ ). We notice that the present alloy has almost the same  $\gamma_{\text{usf}}$  and  $\gamma_{\text{utf}}$ , and a small negative  $\gamma_{\text{isf}}$ , which differs substantially from the case of conventional alloys [36–38]. To obtain an insight into the atomic-level mechanisms behind the trend of the fault energies, we divide  $\gamma$  into three contributions: the chemical part  $\gamma^{\text{chem}}$ , the magnetic part  $\gamma^{\text{mag}}$ , and the electronic part  $\gamma^{\text{el}}$ . It is clear that  $\gamma^{\text{chem}}$  follows closely the trend of  $\gamma$ , while  $\gamma^{\text{mag}}$  gives opposite contributions. Further analysis shows that  $\gamma^{\text{chem}}$  gives the major contribution to the total fault energy (order of  $10^2 \text{ mJ/m}^2$ , especially for  $\gamma_{\text{usf}}$  and  $\gamma_{\text{utf}}$ ). On the other hand,  $\gamma^{\text{mag}}$  plays an important role in establishing the actual values for  $\gamma_{\text{isf}}$  and  $\gamma_{\text{esf}}$  (where  $\gamma^{\text{chem}}$  is relatively small). Finally,  $\gamma^{\text{el}}$  is very small ( $< 10^0 \text{ mJ/m}^2$ ) for the present system and temperatures of interest and thus can safely be ignored.

The magnetic fluctuation contribution is therefore important to identify  $\gamma^{\text{mag}}$  of the paramagnetic FeCrCoNi, as shown in Figure 1(b). In perfect fcc lattice, the local magnetic moments per Fe and Co atoms are  $2.08$  and  $0.32 \mu_{\text{B}}$ , respectively, while for Cr and Ni atoms, the static DLM magnetic moments are nearly zero. For all types of planar fault, the main magnetic changes are observed in the layers around the fault plane. For the intrinsic stacking fault, the Fe magnetic moment near the fault plane decrease by  $\sim 4\%$  as compared to its bulk value. The Co magnetic moment follows qualitatively the same behavior. The loss of the paramagnetic moment results in lower magnetic entropy, and thus has a positive contribution to  $\gamma_{\text{isf}}$ . In the case of the unstable stacking fault, the magnetic entropy is larger than the corresponding bulk values. From the feature of the local magnetic moments, the unstable twinning fault can be treated as a sum of unstable stacking fault and intrinsic stacking fault, and the extrinsic stacking fault as a pair of intrinsic stacking fault located on neighboring planes.

For the considered system, the Curie temperature estimated via the mean-field method [39] varies from  $\sim 155$  to  $\sim 140 \text{ K}$  when  $x$  changes from 0 to 0.3 in the fcc phase [40]. Figure 2(a) displays the obtained  $\gamma_{\text{isf}}$ ,  $\gamma_{\text{usf}}$  and  $\gamma_{\text{utf}}$  of the ferromagnetic and paramagnetic FeCrCoNi in the temperature range of  $77$ – $300 \text{ K}$ . It is clear that for both magnetic states,  $\gamma_{\text{isf}}$  increases, whereas  $\gamma_{\text{usf}}$  and  $\gamma_{\text{utf}}$  decrease with increasing temperature. The values of  $\gamma_{\text{isf}}$  at  $77 \text{ K}$  for the ferromagnetic and paramagnetic states are  $-12.9$  and  $-12.3 \text{ mJ/m}^2$ , respectively, and increase to  $-11.0$  and  $-0.3 \text{ mJ/m}^2$  when temperature

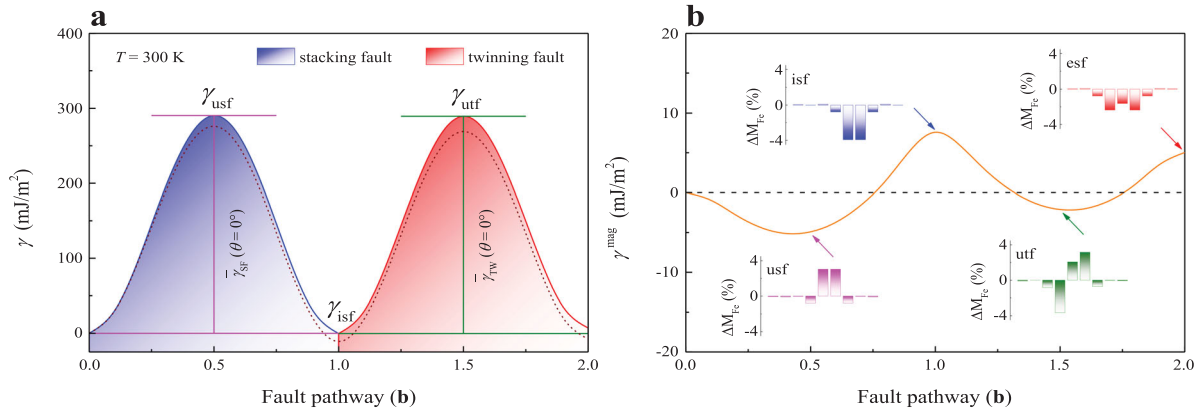


**Figure 1.** Generalized stacking fault energy of the paramagnetic FeCrCoNi at room temperature. In panel (a),  $b = \langle 11\bar{2} \rangle / 6$  is the Burgers vector of the partial dislocation (in units of fcc lattice parameter). For comparison, the dash line marks the  $\gamma$ -surface of the ferromagnetic FeCrCoNi at room temperature. Panel (b) shows the magnetic part  $\gamma^{\text{mag}}$  for the paramagnetic FeCrCoNi at room temperature. Insets show the changes of magnetic moments for Fe around the faulted planes as a function of layer index with respect to the corresponding values for the perfect fcc lattice. The stacking fault is formed between the fifth and sixth layers.

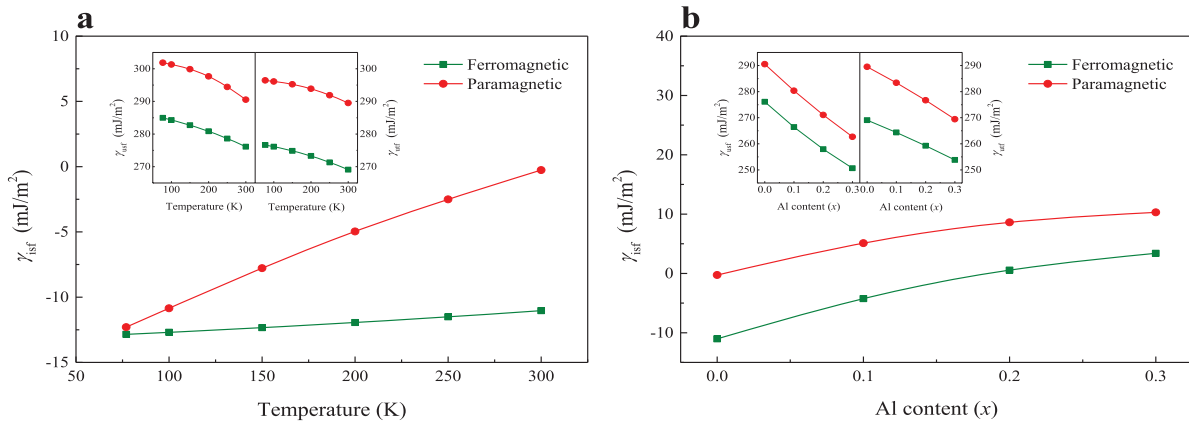


**Figure 2.** Intrinsic stacking fault energy  $\gamma_{\text{isf}}$ , unstable stacking fault energy  $\gamma_{\text{usf}}$ , and unstable twinning fault energy  $\gamma_{\text{utf}}$  of the ferromagnetic and paramagnetic FeCrCoNiAl<sub>x</sub>, respectively. Panel (a) shows the results for FeCrCoNiAl<sub>x</sub> at  $x = 0$  as a function of temperature. Panel (b) shows the results for FeCrCoNiAl<sub>x</sub> at  $T = 300$  K as a function of Al content.

reaches 300 K. The relative large positive temperature factor for  $\gamma_{\text{isf}}$  at the paramagnetic state is mainly contributed by the magnetic part, which has important implication on the deformation mechanism as explained below.

In Figure 2(b), we present the obtained  $\gamma_{\text{isf}}$ ,  $\gamma_{\text{usf}}$  and  $\gamma_{\text{utf}}$  for the ferromagnetic and paramagnetic FeCrCoNiAl<sub>x</sub> at 300 K as a function of Al content. As one can see, removing the magnetic order yields a positive effect on all three parameters within the considered composition range. In the case of the paramagnetic state,  $\gamma_{\text{isf}}$  increases from  $-0.3$  to  $10.3$  mJ/m<sup>2</sup> when  $x$  changes from 0 to 0.3, whereas  $\gamma_{\text{usf}}$  and  $\gamma_{\text{utf}}$  decrease from 290.5 and 289.5 mJ/m<sup>2</sup> to 262.7 and 269.4 mJ/m<sup>2</sup>, respectively. Actually,  $\gamma_{\text{isf}}$  can be connected to the stability of the fcc and hcp structures, i.e.  $\gamma_{\text{isf}} \simeq 2(E_{\text{hcp}} - E_{\text{fcc}})/A$ , based on the second-order approximation of the axial interaction model [22]. Thus, the negative  $\gamma_{\text{isf}}$  found in low-Al

content system at cryogenic temperatures indicates that the fcc structure becomes unstable with respect to the hcp structure.

It is known that in fcc metals, stacking fault (SF), twinning (TW), and full-slip (SL) are important plastic deformation modes [41]. Previous work indicated that the preferred mode is decided by the competition between the corresponding effective energy barriers (EEBs) [42], i.e.  $\bar{\gamma}_{\text{SF}} = \gamma_{\text{usf}} / \cos \theta$ ,  $\bar{\gamma}_{\text{TW}} = (\gamma_{\text{utf}} - \gamma_{\text{isf}}) / \cos \theta$ ,  $\bar{\gamma}_{\text{SL}} = (\gamma_{\text{usf}} - \gamma_{\text{isf}}) / \cos(60^\circ - \theta)$ . Here,  $\bar{\gamma}_{\text{SF}}$ ,  $\bar{\gamma}_{\text{TW}}$  and  $\bar{\gamma}_{\text{SL}}$  denote the EEBs of SF, TW, and SL, respectively, and  $\theta$  measures the angle between the stacking fault easy direction  $\langle 11\bar{2} \rangle$  and the applied resolved shear stress ( $0^\circ \leq \theta \leq 60^\circ$ ). The activated deformation mechanism is decided by the lowest EEBs. For example, TW is preferred over SF when  $\bar{\gamma}_{\text{TW}} < \bar{\gamma}_{\text{SF}}$ , which should be characteristic for metals showing twinning-induced plasticity

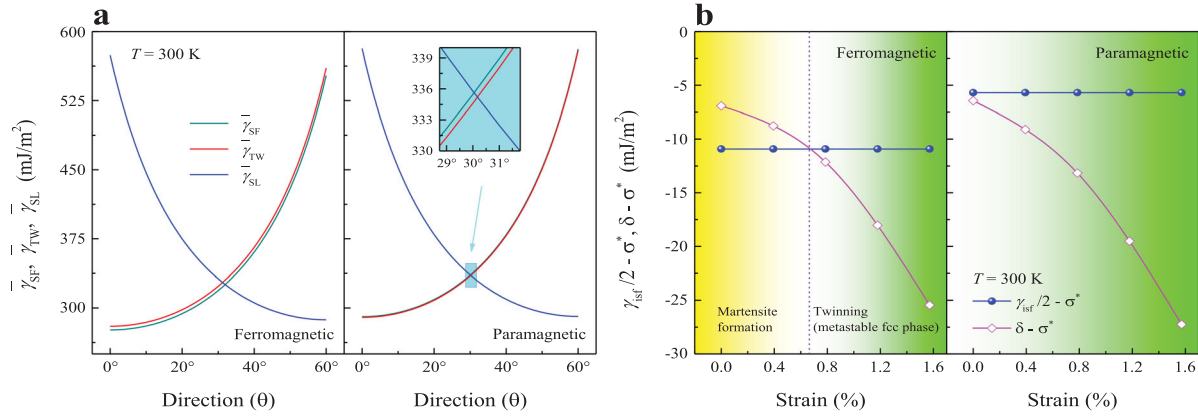


**Figure 3.** Intrinsic material parameters of the ferromagnetic and paramagnetic FeCrCoNi at 300 K. Panel (a) shows the effective energy barriers  $\bar{\gamma}_{SF}$ ,  $\bar{\gamma}_{TW}$ , and  $\bar{\gamma}_{SL}$  as a function of  $\theta$ . Panel (b) shows the twinning parameters ( $\gamma_{isf}/2 - \sigma^*$ ) and ( $\delta - \sigma^*$ ) as a function of affine shear strain.

(TWIP) effect. In Figure 3(a), we present the calculated EEBs of the ferromagnetic and paramagnetic FeCrCoNi at 300 K as a function of  $\theta$ . We notice that the actual value of  $\theta$  does not influence the competition between TW and SF, while at high angle SL mode can always be activated. In the following, we show  $(\bar{\gamma}_{SF} - \bar{\gamma}_{TW}) \equiv \bar{\gamma}_{SF}(0^\circ) - \bar{\gamma}_{TW}(0^\circ)$  for the sake of simplicity, and do not always mention SL when discussing the SF and TW modes.

Some typical multi-component alloys with excellent mechanical properties are reported to be thermodynamically unstable at ambient and cryogenic conditions [4,5,31–35]. Since twinning is recognized as an important deformation mode behind the simultaneous increase of strength and ductility in these alloys, Huang et al. introduced a mechanism of metastable twinning (MTW) based on the stacking fault energies and related intrinsic materials parameters [35]. It was shown that the condition of MTW reads  $\delta < \gamma_{isf}/2 < \sigma^*$ , where  $\sigma^*$  is the pseudo-interfacial energy between the hcp embryo and the fcc matrix [43], and  $\delta \equiv \gamma_{utf} - \gamma_{usf} - \gamma_{isf}/2$  expresses the deviation relative to the so-called universal scaling law [44]. Notice that MTW can only be realized when  $(\delta - \sigma^*) < 0$ , and alloys with  $(\gamma_{isf}/2 - \delta) < 0$  and  $(\gamma_{isf}/2 - \sigma^*) > 0$  represent SF and normal TW, respectively.

The deformation mode is sensitive to the shearing condition in some metastable alloys [35]. The beneficial effect of strain on the twinnability is also mentioned in connection with the empirical deformation maps [41]. We notice that two different types of deformations (alias and affine) have been used in the theoretical investigations [6,45]. For the alias shear, only half of the crystal is displaced in the shearing direction, and the corresponding energy-displacement curve is the  $\gamma$ -surface, as shown in Figure 1. For the affine shear, all atomic planes

are shifted parallel to the shearing direction. In order to illustrate the shearing effect, here we combine these two deformations in the following way: affine shear is applied first in elastic deformation regime, and then alias shear occurs when the critical strain is reached. The shear strain is given by  $|\vec{x}|/h$ , where  $\vec{x}$  is the displacement of the end point of the lattice vector  $\vec{c}$  along the Burgers vector, and  $h$  is the corresponding interlayer spacing.

Figure 3(b) presents the critical MTW parameters ( $\gamma_{isf}/2 - \sigma^*$ ) and ( $\delta - \sigma^*$ ) of the ferromagnetic and paramagnetic FeCrCoNi at 300 K as a function of affine shear strain. It is found that at the ferromagnetic state, SF is the active deformation mode in the low-strain region, and MTW becomes favorable with increasing the affine shear strain. On the other hand, the paramagnetic FeCrCoNi satisfies the MTW condition at all strains from the figure and thus it is prone to MTW. Extending the above study to FeCrCoNiAl<sub>x</sub> ( $0 \leq x \leq 0.3$ ), as shown in Figure 4(a), indicates that SF or MTW can appear at 300 K within the certain composition and magnetic state.

Figure 4(b) presents the composition, temperature, and strain-dependent  $(\bar{\gamma}_{SF} - \bar{\gamma}_{TW})$  of the ferromagnetic and paramagnetic FeCrCoNiAl<sub>x</sub>, respectively. We recall that  $(\gamma_{isf}/2 - \sigma^*) < 0$  implies a thermodynamically unstable fcc phase. Accordingly, normal TW happens only in a high-Al content system or at high temperature (not shown). Within the considered composition and temperature ranges, the MTW (SF) mode occurs with increasing (decreasing) Al content, temperature, and strain, since  $(\bar{\gamma}_{SF} - \bar{\gamma}_{TW})$  is positive (negative) in the right-higher (left-lower) corner of the map. Particularly, magnetism plays an important role in determining the favored deformation mode. For example, the equiatomic FeCrCoNi is predicted to show SF instead of MTW if the alloy remains in the ferromagnetic state at room temperature. The present theoretical results are helpful to explore

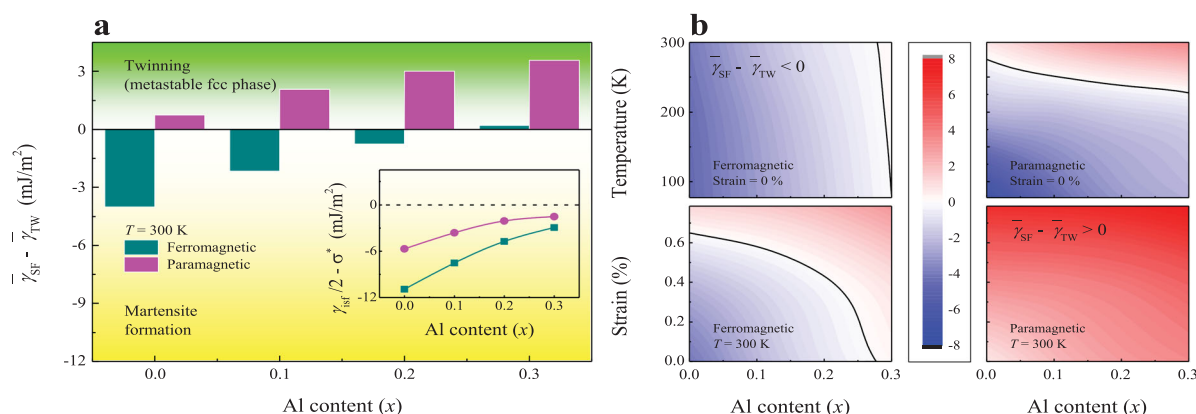


**Figure 4.** Effective energy barriers difference of the ferromagnetic and paramagnetic  $\text{FeCrCoNiAl}_x$  as a function of Al content. Panel (a) shows  $(\gamma_{\text{SF}} - \gamma_{\text{TW}})$  and  $(\gamma_{\text{isf}}/2 - \sigma^*)$  at 300 K. Panel (b) shows  $(\gamma_{\text{SF}} - \gamma_{\text{TW}})$  as a function of temperature and affine shear strain, respectively, and the solid line corresponding  $(\gamma_{\text{SF}} - \gamma_{\text{TW}}) = 0$ . Martensitic transformation and metastable twinning are present within the considered composition and temperature ranges.

alternative ways to tune the plastic flow mechanisms in engineering materials involving HEAs.

The TWIP effect was indeed observed in the considered HEAs at various deformation conditions in experimental, and it was suggested to be the main reason for the measured large work hardenability [10–15]. In addition, smaller twin spacing and larger twin thickness were reported in the as-cast alloy compared with the recrystallized one, i.e. large grain size results in a high twinning activity [13]. Here, we would like to highlight this interesting experimental fact which now gains theoretical support in the mirror of the present data. For example, MTW is predicted in the paramagnetic  $\text{FeCrCoNiAl}_x$  ( $0 \leq x \leq 0.3$ ) at 300 K, which has a Curie point far below room temperature. The good agreement between theory and experiment demonstrates the validity of evaluating the deformation mechanism based on the above criteria.

The combined increase in strength and ductility observed in the recently developed HEAs broadened the palette of advanced metallic materials. A theoretical understanding of the underlying plasticity mechanisms is therefore important for the optimal design and use of these new alloys. In this study, we have investigated the composition and temperature dependence of the generalized stacking fault energy for the ferromagnetic and paramagnetic  $\text{FeCrCoNiAl}_x$  ( $0 \leq x \leq 0.3$ ) HEAs using quantum mechanical first-principle methods. The activation of plastic deformation mechanisms is analyzed by the effective energy barriers in connection with a transparent atomic-level theory of the metastable twinning mechanism. The observed TWIP effect is discussed, and the strain condition exhibits a positive effect on the twinnability. Theory predicts that the TRIP phenomena become the favored deformation mode in low-Al content system and at cryogenic conditions. The disclosed

behavior of the present HEAs demonstrates that a proper control of the magnetic state offers a way to identify alloys with a change in the main activated plastic deformation modes, which can facilitate the design and optimization of alternative HEAs with desired strength-ductility combinations.

## Disclosure statement

No potential conflict of interest was reported by the authors.

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