



# Computational thermodynamic and first-principles calculation of stacking fault energy on ternary Co-based alloys



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## ABSTRACT

Theoretical calculation of stacking fault energy (SFE) needs to be investigated closely in each alloy system due to the complex effect between different elements. In this study, we have revealed that the computational thermodynamic approach and first-principles density-functional-theory (DFT) calculations are capable of calculating the SFE for developing and designing ternary Co-based alloys with low SFE and excellent mechanical properties. Interaction between Ni and Cr atoms in ternary systems can make a distinct effect to the SFE while interaction between Cr and Mo atoms gives more charge transfer than lower the SFE. Effect of alloying atom position and Cr concentrations of Co–Cr–W alloys was studied and explained regarding the electronic structure. In high Cr concentrations, Cr atoms that dispersing uniform are more useful to improving the strengthening effect than those dispersing segregatively.

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## 1. Introduction

Computational thermodynamic and first-principles methods play an important role in developing and designing Co-based alloys, Ni-based alloy, Mg-based alloy, shape memory alloys and 3rd generation Advanced High Strength Steel (AHSS) through stacking fault energy (SFE) modeling [1–5]. The advantages of these theoretical methods are; can provide fundamental understanding of the complex effect between the different elements on the SFE, can calculate a whole concentration to provide insights on general trends, the computational effort can minimize, and by first-principles methods, it can calculate a highly accurate SFE modeling (including unstable SFE) without any experimental data [1,4]. However, there are inconsistencies in the published literature regarding the influence of alloying elements on SFE that may arise from the differences in chemical concentrations and techniques employed [6]. Then, it needs to be investigated closely in each alloy system (binary, ternary, etc.) in order to be fully understood by theoretical calculations. For example, alloying with Ni and Cr increase the SFE of Fe–Mn alloys but have the inverse effect for carbon steels [4].

Intrinsic or stable SFE of binary Co-based alloys has been investigated in our previous work by computational thermodynamic

and first-principles method [1,2,7]. It concludes that the addition of some transition metal (Cr, Mo, W, Re, Os, Ir) and rare-earth (Sc, Y, La, Sm) alloying elements would decrease SFE of pure Co [7] while adding Ni, Mn, Fe and also Al into Co matrix will increase SFE. The effect on the SFE becomes stronger with the increase of alloying elements concentration until 20 at.% for some binary Co-based alloys [2]. In ternary Co-based alloys, the effect of some alloying element to the SFE is similar to the binary system. For example, the effects of Cr, W and Mo addition are reported to decrease the SFE of Co–Cr–X ternary alloys, while the addition of Ni increase SFE and reduces a tendency to form stacking faults [8–10]. But there are some inverse effects due to the complex effect or interactions between the alloying elements in the ternary system. For example, the addition of tungsten until 8 wt% in Co–20 wt.%Cr–W alloy will decrease the stacking fault density (increase SFE) [10,11]. To understand the complicated interactions of different elements in ternary Co-based alloys, we investigate the intrinsic SFE of Co–Ni–Cr, Co–Ni–W, Co–Cr–W, Co–Cr–Mo and Co–Al–W alloys by both computational thermodynamic and first-principles methods. SFE of ternary Ni-based alloys have been studied using an integrating CALPHAD (calculation of phase diagram) approach and first-principles by Shang et al [3], and for Mg–Al–Zn alloys by first-principles method [5] while Jiang [12] examined the phase stability of  $L1_2\text{-Co}_3\text{Al}_{0.5}\text{W}_{0.5}$  compound in the Co–Al–W ternary system by first-principles special quasi-random structure (SQS) calculations. Our investigation also explains the interactions of dif-

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ferent elements, the effect of alloying atom position and Cr concentrations of Co-Cr-W alloys regarding the charge density difference distributions and density of states (DOS). This study would be useful for the design of ternary Co-based alloys with low SFE and excellent mechanical properties.

## 2. Computational methodology

The computational thermodynamic of SFE is calculated based on Olson and Cohen [2,13] formulation:

$$\gamma_{sf} = 2\rho\Delta G^{\gamma-\varepsilon} + 2\sigma^{\gamma/\varepsilon} \quad (1)$$

where  $\gamma_{sf}$  is the intrinsic SFE ( $\text{mJ}/\text{m}^2$ ) of the stacking fault,  $\Delta G^{\gamma-\varepsilon}$  is the Gibbs free energy difference of the transformation of  $\gamma$ -fcc to  $\varepsilon$ -hcp phase, and  $\sigma^{\gamma/\varepsilon}$  is the interfacial energy per unit area of the phase boundary which is assumed to be a constant value ( $\sigma^{\gamma/\varepsilon} = 7.5 \text{ mJ}/\text{m}^2$ ). Full descriptions of the present calculations were presented in Reference [2] and in [Supplementary material](#). The thermodynamic data for the calculations were taken from the data published by Scientific Group Thermodata Europe (SGTE) [14] and from publications of computational thermodynamic approach of phase equilibria studies (CALPHAD) [2]. It is important to note that beside the binary interaction parameter, there is the ternary excess Gibbs free energy  ${}^E G_{ij,k}^{\gamma-\varepsilon}$  that can be essential to the SFE value of ternary system. Due to limited available data reported, then not all the ternary system used the ternary excess Gibbs free energy data. The influence of Al and Mo additions on the magnetic moment was not taken into consideration and no ternary magnetic parameter are applied. All the thermodynamic data were applied into a Matlab code which was encoded for the SFE calculations of ternary Co-based alloys.

The first-principle calculation of SFE is calculated based on the supercell method;

$$\gamma_{sf} = \frac{E_{isf} - E_0}{A} \quad (2)$$

where  $E_{isf}$  is the total energy of the supercell with intrinsic stacking fault,  $E_0$  is the total energy of the ideal fcc structure without stacking fault, and  $A$  is the area of the stacking fault plane (varied according to the equilibrium lattice constant  $a_0$  of the supercell). The supercell consists of 22 atoms with 11 layers and ABCABCABCAB stacking sequence of close-packed (1 1 1) planes as the ideal structure, then displacement of the layers number 7–11 along [1 1 -2] will create the intrinsic stacking fault (ISF) supercell ABCABC [BCABC [2]. All supercells separated from the rest by an 8 Å vacuum to avoid interaction between periodic images in the [1 1 1] direction due to periodic boundary conditions. We calculated the total energy of the supercells using the CASTEP package [15] based on density-functional theory (DFT) [16] with the Perdew–Burke–Ernzerhof (PBE) [17] version of the generalized gradient approximation (GGA) and the ultrasoft pseudopotential initiated by Vanderbilt [18] after fully relaxing the structure. The convergence parameters as follows: total energy tolerance  $10^{-5}$  eV/atom, force tolerance 0.03 eV/Å, maximum stress 0.05 GPa and maximum displacement 0.001 Å. The Monkhorst-Pack [19] scheme k-points grid sampling is set as 36 irreducible k-points ( $11 \times 11 \times 1$ ) in the Brillouin zone and the plane wave energy cut-off is 400 eV. The calculations used a spin-polarized setting that uniformly distributed over the space of the alloying atoms. Our previous work shows that it is reasonable to calculate the SFE with different alloying elements only using 11 layers with 22 atoms [1,2].

The alloying atoms selected in this study are forming solid solutions in alloys based on binary and ternary Co-based alloys phase diagrams [2], then treatment of the chemical disorder required careful consideration. It can be solved by using special quasiran-

dom structures (SQS) that represent the best periodic supercell approximation to the true disordered state for a given number of atoms per supercell [11]. Then, it would require multiple calculations to determine average SFE. To reduce the computational complexity and since the main assumption of the SFE formation by computational thermodynamic is basically a thin layer of hcp phase in an fcc crystal [13], then the alloying atom position in the supercells structure is ordered in the stacking fault region to represent ternary solid solutions. It is believed that substitutional alloying atoms are attracted to a stacking fault region (Suzuki effect) from the experiment by Han et al. [20] in Co-Ni-Cr based superalloy MP159. Therefore, alloying atoms are usually assumed to reside in the stacking fault layer in the SFE calculation [1–3]. In this study, two kinds of alloying atoms substitute two cobalt atoms in 5th and 7th layers with low-energy positions, then the concentration of alloying atoms was about 4.5 at.%. We also compared the SFE of two different structures of ternary Co-Cr-W alloys and analyze the effect of the alloying atom positions. In fact that the total energy difference ( $E_{isf} - E_0$ ) is used in the SFE calculation, the SFE differences obtained by different structures is relatively small.

## 3. Results and discussions

### 3.1. SFE of ternary Co-based alloys

The calculated intrinsic SFE of ternary Co-based alloys by the computational thermodynamic approach are shown in Fig. 1. In Co-Ni-Cr alloys (Fig. 1(a)), alloying with Cr atom (from 0 until 5 at.%) significantly decrease SFE in all range of Ni contents from -9 to  $-20 \text{ mJ}/\text{m}^2$ . Meanwhile, alloying with Ni atom slightly increase SFE when Cr contents are lower than 3 at.%, but when Cr contents are higher than 3 at.%, increasing Ni concentrations slightly decrease SFE. This result indicates that interaction between Ni and Cr in ternary systems can make a distinct effect to the SFE, in contrast to the effect of an alloying atom in binary Co-Cr or Co-Ni alloys alone [1,2]. Modification of Cr with W in Co-Ni-W alloys as shown in Fig. 1 (b), the SFE is more decrease than Co-Ni-Cr alloys ( $-10$  to  $-28 \text{ mJ}/\text{m}^2$ ) with the increase of W contents while increasing Ni contents slightly increase SFE in all range due to no interaction between Ni and W. Then, in Co-Cr-W alloys (Fig. 1(c)), both alloying with Cr and W will decrease SFE in all range from  $-11$  to  $-42 \text{ mJ}/\text{m}^2$ . The SFE is more decrease with the increase of Mo content in Co-Cr-Mo alloys from  $-11$  to  $-94 \text{ mJ}/\text{m}^2$  (Fig. 1(d)). In Co-Al-W alloys (Fig. 1(e)), the SFE decrease from  $-1$  to  $-29 \text{ mJ}/\text{m}^2$  by decreasing Al contents and increasing W contents. From the computational thermodynamic approach, alloying atoms that significantly decrease the SFE of ternary Co-based alloys are Ni, Cr, W and Mo, respectively.

The calculated SFE by first-principles are presented in Table 1 together with the computational thermodynamic approach and SFE differences. By fitting the total energy versus volume (E-V) data points according to the 4-parameter Murnaghan equation of state (EOS), we determine the equilibrium lattice parameter ( $a_0$ ) and equilibrium volume ( $V_0$ ). The result of pure Co has been compared with another DFT calculation and experimental values in our previous study and shows a good agreement [1,2]. Substituting Co atom by alloying atom will induce lattice or volume expansion. Ternary Co-based alloys with larger equilibrium volume and lattice parameter than pure Co tend to decrease the SFE as shown in Table 1. The sequences of the SFE of ternary Co-based alloys with 4.5 at.% alloying atoms are as follows; Co-Ni-Cr > Co-Ni-W > Co-Ni-W > Co-Cr-W > Co-Cr-Mo. This sequence is similar to the computational thermodynamic result and the SFE differences are relatively small. Reasons for the deviations that involved in SFE

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