



First-principles study on the stability of interstitial carbon and nitrogen and their influence on the plastic deformation mechanisms in a Co–Cr–W–Ni quaternary alloy

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ABSTRACT

Carbon (C) and nitrogen (N) are critical elements for improving the mechanical properties of Co–Cr-based biomedical alloys and medium/high-entropy alloys. However, owing to the complex local atomic configurations in multicomponent alloys, the effects of interstitial C/N elements on the generalized stacking fault energy (GSFE) and underlying plastic deformation mechanisms remain poorly understood. In this study, we investigated the stability of interstitial C/N atoms and their effects on the GSFE of a Co–Cr–W–Ni quaternary alloy using first-principles calculations combined with special quasi-random structures and supercell methods. Formation energy analyses revealed that, relative to Co, the presence of W and Ni in the first nearest-neighbor shell tends to destabilize the C/N atoms, whereas Cr acts as a stabilizer. N exhibits pronounced stabilization by Cr, suggesting the formation of Cr–N short-range order (SRO). Furthermore, GSFE analysis demonstrated that both C and N addition increased the intrinsic stacking fault energy. The addition of C and N also tended to enhance twinning-ability. N addition is expected to provide a greater increase in yield strength than C addition owing to SRO formation. Both C and N additions are expected to suppress the γ -to- ϵ strain-induced martensitic transformation, a mechanism known to contribute to higher ductility. Simultaneously, the promotion of deformation twinning suggests a potential pathway toward an exceptional balance of ultimate tensile strength and ductility, providing valuable insights for advanced alloy design.

1. Introduction

The face-centered cubic (fcc, γ) Co–25Cr–5W–11Ni (mol%, ASTM F90, CCWN) alloy [1] exhibits excellent corrosion and wear resistance, an optimal balance of strength and ductility, and favorable biocompatibility, making it widely used as a platform alloy for balloon-expandable stents [2–4]. To facilitate minimally invasive medical treatments and suppress restenosis, there is a growing demand for stents with thinner struts and smaller diameters [5–7]. This requires constituent materials that maintain a low yield strength while concurrently exhibiting high ultimate tensile strength (UTS) and high ductility. The mechanical properties of biomedical Co–Cr–Mo alloys have typically been improved through the addition of interstitial elements such as carbon (C) and nitrogen (N) [8,9]. Furthermore, the CCWN quaternary alloy is classified as an fcc medium-entropy alloy (MEA). In the field of multicomponent alloys, such as MEAs and high-entropy alloys (HEAs), improved

mechanical properties via the addition of C and/or N have been widely reported as an effective alloy design strategy [10–15]. Therefore, understanding how C and N additions affect the plastic deformation of CCWN quaternary alloys is crucial for optimizing stent materials, which are used in plastically deformed states, and for clarifying the role of interstitial-element doping in the mechanical properties of multicomponent alloys.

The stacking fault energy (SFE) of fcc alloys directly affects their mechanical properties. As the SFE increases, the primary plastic deformation mechanism transitions from γ -to- ϵ strain-induced martensitic transformation (SIMT) to deformation twinning, and subsequently to dislocation slip [16,17]. Activating transformation-induced plasticity (TRIP) or twinning-induced plasticity (TWIP) promotes work hardening, leading to high UTS and ductility [15,18]. C is known to increase the SFE of Co-based alloys [9]. N stabilizes the γ -phase [8,19–25]; however, the specific influence of N on SFE varies depending on the alloy system and

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remains unclear. For example, Li et al. [23] reported that N addition to a Co–Cr–Mo alloy improves γ -phase stability by elevating the energy barrier for the γ -to- ϵ phase transformation, rather than thermodynamically stabilizing the γ -phase. Conversely, in CoCrFeNiMn [26] and Co₂₀Cr₂₀Fe₃₀Mn₂₄Ni₆ [11] HEAs, both first-principles calculations and experimental measurements indicated that N addition increased the SFE.

Experimentally, transmission electron microscopy (TEM) has been widely used to evaluate SFE [11,27,28]. However, in high-SFE alloys, the narrow width of extended dislocations makes accurate measurements challenging [29,30]. As an alternative, first-principles calculations based on density functional theory (DFT) have been increasingly used [31–33]. An effective approach involves calculating the generalized stacking fault energy (GSFE) by directly introducing a dislocation into the crystallographic plane within a supercell. This method quantifies the energy barriers during continuous plastic deformation, thereby helping identify the dominant plastic deformation mechanisms [34–36]. Nevertheless, GSFE analyses evaluating the effects of C and N have primarily focused on pure metals, such as Fe and Ni [37,38], where interstitial sites are surrounded by uniform host atoms. By contrast, modeling multicomponent solid solutions via DFT requires the use of special quasi-random structures (SQS) [39,40]. To accurately assess the effect of C/N on the GSFE of multicomponent alloys, it is necessary to consider how the local atomic configurations affect the stability of the interstitial sites. Although C and N are known to occupy octahedral sites in fcc alloys [12,41,42], first-principles studies on interstitial-element effects in multicomponent alloys have mostly relied on indirect methods that estimate SFE by comparing the phase stabilities of fcc, hexagonal close-packed (hcp), and double-hcp structures (e.g., the axial nearest-neighbor Ising model or the axial next-nearest-neighbor Ising model) [11,12,41,42,43]. In other words, few studies have identified the stable sites of interstitial elements in multicomponent alloys by accounting for local atomic configurations and subsequently analyzed the GSFE through direct shear deformation to elucidate the influence of interstitial-element additions on plastic deformation mechanisms.

In our previous study [44], we combined the SQS and supercell methods to investigate the stability of C/N and their effects on the GSFE in Co–X (X = Cr, W, Ni) binary alloys, which constitute subsystems of the CCWN quaternary alloy. We demonstrated that one C/N atom is stable in an octahedral site and analyzed how the local composition and atomic configuration of these octahedra govern their stability. By applying the single diffusion hop mechanism [45,46], we showed that it is energetically favorable for a C/N atom to migrate to an adjacent octahedral site during plastic deformation. Furthermore, we established that the effects of C/N on the GSFE can be effectively evaluated by incorporating the octahedral site containing C/N into the generalized stacking fault (GSF). Experimentally, we have also reported that the addition of C to the CCWN quaternary alloy increases its UTS and plastic elongation [47]. However, because of the complex local composition and atomic configuration of the CCWN quaternary system, the stable sites for C and N, as well as their effects on the GSFE and plastic deformation mechanisms, remain unclear. Therefore, in the present study, we employ first-principles calculations combining the SQS and supercell methods to investigate the CCWN quaternary alloy. We first use multiple regression analysis to systematically evaluate how the local compositions and atomic configurations of the octahedral sites affect the stability of one C/N interstitial atom. Finally, through GSFE analysis, we clarify the effect of C/N additions on the plastic deformation mechanisms of the CCWN quaternary alloy.

2. Materials and methods

2.1. Alloy model

The alloy model and computational methodology employed in this study have been described in detail elsewhere [34,44]. Accordingly,

only a brief overview is provided here.

An fcc primitive-cell-based $4 \times 4 \times 9$ supercell comprising a total of 144 metallic atoms was constructed as the alloy model. The supercell consists of nine atomic layers stacked along the [111] crystallographic direction. Each layer contains 4×4 atoms. The layers are sequentially numbered from the bottom (first layer) to the top (ninth layer).

The SQS model [39,40] was adopted to represent the random atomic configurations of the alloys. The validity of the SQS approach for evaluating phase stability in multicomponent alloy systems has been well established in our previous studies [48–50].

The composition of the alloy model was determined based on the commercial ASTM F90 alloy [1] (Co–25Cr–5W–11Ni, mol%). Table 1 summarizes the number of atoms in the supercell used in this study and the corresponding elemental composition (mol%). Because one C/N atom was added to the 144 metallic atoms, the C or N content corresponded to approximately 0.7 mol%. The models were designated as CCWN-without, CCWN-C, and CCWN-N depending on the presence or absence of C/N. Fig. 1 illustrates the supercell of the CCWN-without model.

2.2. Introduction of C/N

One C/N atom was placed at an octahedral site as an interstitial atom. The CCWN-without model contained 144 octahedral sites. The formation energies of solute C/N in the CCWN quaternary alloy, E_{formX} (X = C or N), were calculated by placing one C/N atom at each of these 144 sites and performing full structural relaxation. The equation for calculating E_{formX} is as follows:

$$E_{\text{formX}} = E_{\text{withX}} - E_{\text{withoutX}} - E_{\text{C/N}} \quad (1)$$

where E_{withX} is the total energy of the CCWN-C or CCWN-N model, and E_{withoutX} is the total energy of the CCWN-without model. The values used for $E_{\text{C/N}}$ were identical to those in [44], and they indicate the total energy of one C atom with a graphene structure or half the total energy of an N₂ molecule.

2.3. Introduction of GSF

Following the calculations of E_{formX} , GSFE calculations were performed on the interlayers containing the most stable octahedral sites for C/N (each interlayer comprised 16 octahedral sites). To evaluate the effect of C/N addition on the GSFE, the interlayers containing C/N were rearranged to be positioned as the fifth and sixth layers, while maintaining the relative positions of the SQS. To directly compare the effects of C and N addition on the GSFE, calculations were performed for configurations in which the C and N atoms were exchanged. Consequently, the GSFE was evaluated by placing C and N at 32 octahedral sites (16 sites $\times$ 2 interlayers) for each C/N.

After an initial full structural relaxation, a vacuum layer of 10 Å was introduced along the [111] direction to eliminate interatomic interactions from the three-dimensional periodic boundary conditions. The Burgers vector was set to $b_p = \frac{[11\bar{2}]}{6}a$, where a is the lattice constant, and the shear increment was defined as $0.5|b_p|$.

Table 1

Numbers of atoms and composition (mol%) of CCWN quaternary alloy models with and without C/N addition.

Co–Cr–W–Ni quaternary models		Element					
Model name		Co	Cr	W	Ni	C	N
CCWN-without	Number	84	36	8	16	0	0
	mol%	58.3	25.0	5.6	11.1	–	–
CCWN-C	Number	84	36	8	16	1	0
	mol%	57.9	24.8	5.5	11.0	0.7	–
CCWN-N	Number	84	36	8	16	0	1
	mol%	57.9	24.8	5.5	11.0	–	0.7

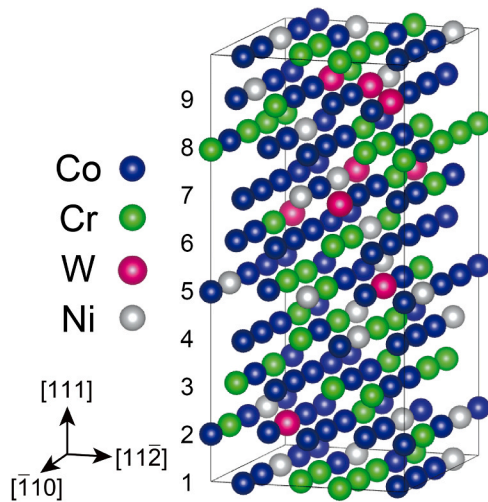


Fig. 1. Appearance of a $4 \times 4 \times 9$ supercell of the CCWN-without model.

Fig. S1 in the [supplementary material](#) illustrates the introduction of the GSF. We introduced the GSF in two steps. Initially, shearing the upper section (from the sixth to ninth layers) along the $[1\bar{1}2]$ direction produced an unstable stacking fault (USF) ($0.5|b_p|$) and an intrinsic stacking fault (ISF) ($1.0|b_p|$). Subsequently, the shearing of the lower section (from the first to fourth layers) along the $[11\bar{2}]$ direction produced an unstable twin fault (UTF) ($1.5|b_p|$) and an extrinsic stacking fault (ESF) ($2.0|b_p|$).

Concurrently, the displacement of the C/N atoms during the introduction of the GSF was determined based on the single diffusion hop mechanism. Although the applicability of this mechanism has not been experimentally verified for Co–Cr–W–Ni quaternary alloys, it was adopted, as described in the Introduction, based on a computational study of Co–X binary alloys [44] and on experimental and computational studies of TWIP steels [45,46]. For the USF and ISF, one C/N atom was displaced by $-0.25b_p$ and $-0.5b_p + b_D$ ($b_D = \pm \frac{[110]}{4}a$), respectively. Fig. S2 illustrates the atomic displacements between the fifth and sixth layers, viewed along the $[111]$ direction, during the introduction of the ISF. Following the single diffusion hop mechanism, the C/N atom was positioned at the nearest octahedral site by applying a displacement of b_D . The sign ($\pm$) of this displacement arises from the presence of two nearest-neighbor octahedral sites on the interlayer. To ensure that the C/N atom was positioned at a relatively stable octahedral site, the sign was determined based on the regression equations presented later (Eqs. (5) and (6) for C and N, respectively).

The structural relaxation conditions are color-coded in Fig. S1. The grey layers were fixed. Because the local combinations of atomic bonds in this multicomponent alloy change upon the introduction of the GSF, the pink regions, comprising the GSF and its adjacent layers, were fully relaxed, whereas the green regions were relaxed only along the $[111]$ direction. Conversely, for the USF and UTF, structural relaxation was restricted solely to the $[111]$ direction to prevent the collapse of these unstable structures. Following displacement of the C/N atom via the single diffusion hop mechanism, full structural relaxation was performed in the pink regions (the 4th–7th layers for the ISF and the 3rd–7th layers for the ESF). Out-of-plane movement and migration to another octahedral site were therefore computationally permitted for the C/N atom during the formation of the ISF and ESF. However, such movements did not actually occur; the configuration of the alloying elements in the 1NN shell of the C/N atom was confirmed to remain unchanged before and after structural relaxation.

The formula for calculating GSFE (γ_{GSF}) is expressed as follows:

$$\gamma_{\text{GSF}} = \frac{E_{\text{GSF}} - E_0}{A} \quad (2)$$

where E_{GSF} is the total energy of the system containing a GSF, E_0 is the total energy of a perfect crystal without a GSF, and A is the area of the generalized stacking-fault plane.

2.4. First-principles calculation

All calculations were performed within the DFT framework as implemented in the Vienna Ab-initio Simulation Package (VASP) [51, 52]. The electron-nuclei interactions were described using the projector augmented-wave method [53], while the exchange-correlation functional was treated via the generalized gradient approximation employing the Perdew-Burke-Ernzerhof formula [54]. This standard generalized gradient approximation (GGA) functional was selected to account for local atomic configurations. The Hubbard-corrected GGA approach (GGA+ U), which is widely used to describe the electronic states of transition metals with strongly correlated electrons [55], was not employed to avoid ambiguities associated with empirical parameter fitting; this choice should be recognized as a limitation of the present study. A systematic comparison of GGA and GGA + U results (e.g., lattice constants and magnetic moments) for this system will be pursued in future work. Spin polarization calculations were performed. A ferromagnetic (FM) configuration was adopted based on its energetic stability: the nonmagnetic (NM) configuration, used here as a practical approximation to a paramagnetic state, was higher in energy by $6.6 \text{ meV} \cdot \text{atom}^{-1}$ than the FM configuration. Furthermore, structural relaxation initiated from an antiferromagnetic (AFM) configuration converged to a state with nearly identical energy and local magnetic moments to the FM configuration. These results indicate that the FM state is the most energetically stable magnetic configuration for this alloy system, consistent with exchange interactions among transition-metal 3d electrons. Based on preliminary convergence tests, the plane-wave cutoff energy was set to 500 eV, and the Brillouin zone was sampled using a $4 \times 4 \times 1$ k -point mesh. To eliminate artificial periodic interactions across the introduced vacuum layer, k -point sampling along the $[111]$ direction was restricted to a single point. The convergence criterion for structural relaxation was set to $10^{-4} \text{ eV/system}$ for energy and $0.05 \text{ eV} \cdot \text{\AA}^{-1}$ for force. For the CCWN-without model, the calculated average partial magnetic moments were 0.714 ± 0.384 , -0.269 ± 0.416 , -0.105 ± 0.047 , and $0.170 \pm 0.101 \mu_B \cdot \text{atom}^{-1}$ for Co, Cr, W, and Ni, respectively, giving a total magnetic moment of $52.173 \mu_B$ for the 144-atom supercell. While phonon calculations are often used to assess dynamical stability, they were omitted in this study because the stability of the fcc phase in CCWN quaternary alloys is already well-established experimentally [5,6,47].

3. Results and discussion

3.1. Elastic and electronic interactions induced by the introduction of C/N

The lattice constants for the CCWN-without, CCWN-C, and CCWN-N models were 3.536 , 3.541 ± 0.019 , and $3.542 \pm 0.016 \text{ \AA}$, respectively. The addition of C and N increased the lattice constant at a similar rate of $\sim 0.008 \text{ \AA} \cdot \text{mol}^{-1}$. These values are consistent with previous experimental reports on fcc CoCrFeNiMn HEAs (C addition [56]: $\sim 0.009 \text{ \AA} \cdot \text{mol}^{-1}$; N addition [57]: $\sim 0.008 \text{ \AA} \cdot \text{mol}^{-1}$), thereby validating the present computational models.

Numerous configurations of alloying atoms are possible for octahedral sites in multicomponent alloys, suggesting that the configuration of alloying atoms over a wide region surrounding the C/N atom may affect the stability of C/N. Therefore, elastic and electronic interactions between C/N and alloying atoms were discussed by focusing on alloying atoms up to the third-nearest-neighbor (3NN) shell. Fig. 2 shows the distances between the interstitial atoms (C/N) and surrounding alloying atoms (Co, Cr, W, and Ni) in the first-, second-, and third-nearest-neighbor (1NN, 2NN, and 3NN) shells across the 144 sites for each

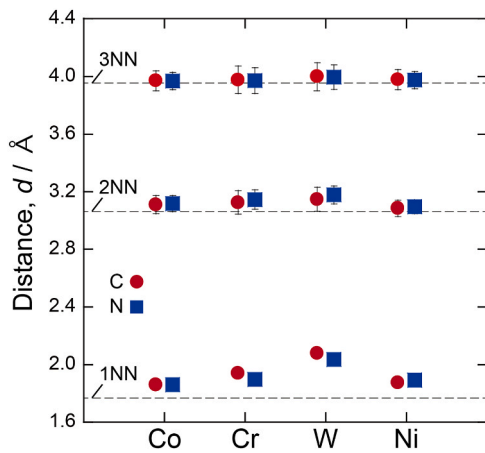


Fig. 2. Distances between the interstitial atom (C/N) and alloying atoms (Co, Cr, W, Ni) of the 1NN, 2NN, and 3NN shells. The dashed lines represent the average distances from the center of the octahedral site to the 1NN, 2NN, and 3NN shells in the CCWN-without model.

alloying element.

The black dashed lines represent the average distances from the center of the octahedral site to the 1NN ($\frac{a}{2} \approx 1.77 \text{ \AA}$), 2NN ($\frac{\sqrt{3}}{2}a \approx 3.06 \text{ \AA}$), and 3NN ($\frac{\sqrt{5}}{2}a \approx 3.95 \text{ \AA}$) shells in the CCWN-without model. Regardless of whether C or N was introduced, the distances between the interstitial atom and neighboring alloying atoms in the 1NN shell showed larger variations for W and Cr than for Co and Ni. Although the distances to W and Cr in the 1NN shell increased more with C addition than with N addition, the distances in the 2NN shell increased more with the addition of N. Because the overall macroscopic increase in the lattice constant was almost identical for C and N, this indicates that the macroscopic elastic lattice distortions are similar, but the local lattice distortion varies depending on the specific interstitial atom and the surrounding alloying elements. In general, changes in the distances near the 3NN shell were minimal for both C and N. This demonstrates that the lattice distortion induced by the introduction of C/N is predominantly governed by local expansion between the interstitial atom and the 1NN shell.

Bader charge analysis [58,59] was performed to evaluate the electronic interactions. As in a previous study [44], the variation in charge was obtained by subtracting the charges of the CCWN-without model and the isolated C or N atom from those of the corresponding CCWN-C or CCWN-N model. Fig. 3 illustrates the relationship between the variation in charge in the unit of e and the distances between the interstitial C/N atom and the alloying atoms in the 1NN, 2NN, and 3NN shells. In the

1NN shell, the alloying atoms lost electrons, exhibiting a variation in charge of approximately -0.15 to -0.4 e , whereas the values in the 2NN and 3NN shells were close to zero. Within the 1NN shell, the variation in charge for both C and N followed the order of $\text{Cr} > \text{Co} > \text{Ni} > \text{W}$. Based on Figs. 2 and 3, we can conclude that the elastic and electronic interactions induced by the introduction of one C/N atom were predominantly localized between the interstitial atom and the 1NN shell.

3.2. 1NN shell configuration dependence on C/N stability

Focusing on the interaction between the C/N atom and 1NN shell, we investigate the stable sites for C/N in the CCWN quaternary alloy. The average E_{formX} values for C and N were 0.30 ± 0.18 and $-0.36 \pm 0.32 \text{ eV}$, respectively, while the minimum values (i.e., at the most stable octahedral sites) were -0.12 and -1.19 eV , respectively. Fig. 4 illustrates the atomic configurations up to the 1NN shell for the most stable octahedral sites of C and N.

When there are two types of alloying atoms, A (a major element) and B (a minor element), there are six possible combinations of octahedral sites in the 1NN shell [41]. For a composition of four A and two B atoms, the configurations are distinguished as cis and trans; for three A and three B atoms, they are distinguished as facial (fac) and meridional (mer). Schematics and abbreviations of these configurations are shown in Fig. S3. As shown in Fig. 4, C was most stable at the 3Co-3Cr-fac site, whereas N was most stable at the 4Cr-2Co-trans site. Notably, the 4Cr-2Co-trans site for N contained the largest number of Cr atoms in the 1NN shell among all octahedral sites in the SQS model used in this study. Fig. 5 shows the charge density difference (CDD) up to the 1NN shell when C or N atom was placed at the most stable octahedral sites for C and N, as shown in Figs. 5(a) and (b), respectively.

At each site, panels 1–4 show the results for C addition, while panels 5–8 show the results for N addition. Furthermore, panels 1, 2, 5, and 6 display the three-dimensional (3D) CDD maps, whereas panels 3, 4, 7,

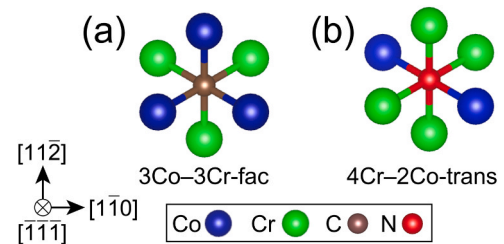


Fig. 4. Atomic configurations of the most stable octahedral sites for (a) C and (b) N atom.

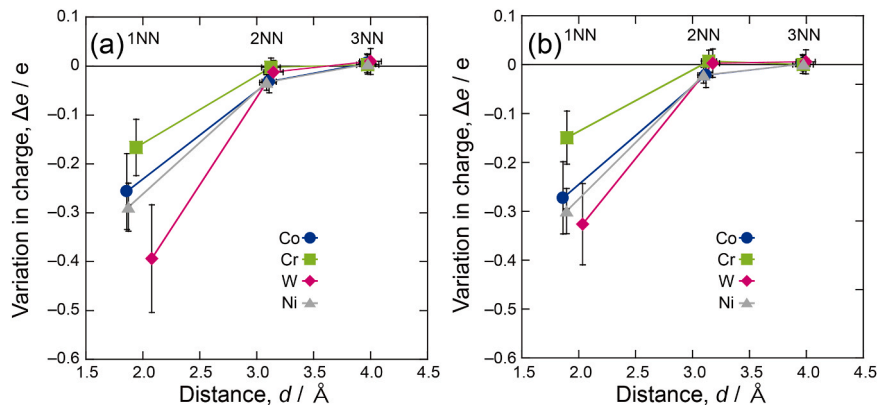


Fig. 3. Relationship between the variation in charge and the distances between the interstitial (a) C or (b) N atom and alloying atoms in the 1NN, 2NN, and 3NN shells.

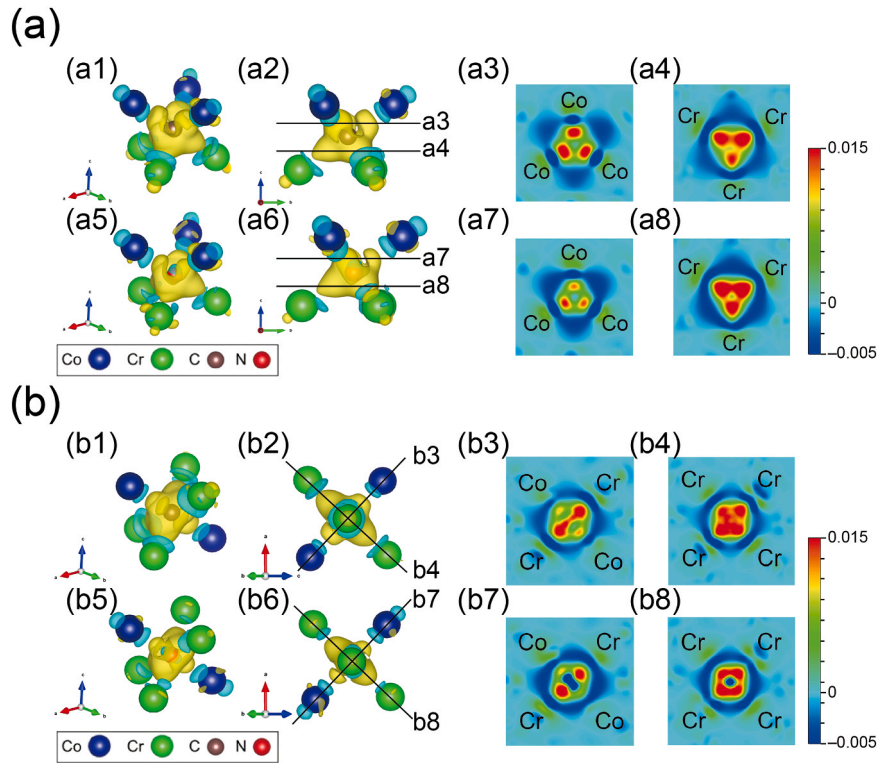


Fig. 5. CDD up to the 1NN shell when C or N was placed at the two most stable octahedral sites. (a) and (b) correspond to the most stable sites for C and N, respectively. For each site, panels 1–4 and 5–8 display the results for the C and N additions, respectively. Panels 1, 2, 5, and 6 represent the 3D CDD maps, where yellow and light blue isosurfaces indicate charge accumulation and depletion, respectively. Panels 3, 4, 7, and 8 show the extracted 2D CDD cross-section maps in unit of e.

and 8 present the corresponding two-dimensional (2D) cross-sectional CDD maps. As shown in the 3D CDD image in Fig. 5(a), this atomic arrangement corresponds to the 3Co–3Cr-fac configuration shown in Fig. 4(a), characterized by a structure where the three Co and three Cr atoms are separated to opposite sides. Corresponding to this local atomic configuration, the yellow regions indicating charge accumulation appear to extend more toward the Cr side than toward the Co side. The 2D CDD further confirmed a more pronounced charge increase in the region adjacent to Cr than to Co, demonstrating that both C and N formed stronger covalent bonds with Cr than with Co. As shown in Fig. 5(b), this atomic arrangement corresponds to the 4Cr–2Co-trans configuration shown in Fig. 4(b), where the local structure consists of four Cr atoms arranged coplanar to the axis connecting the two Co atoms. In the 3D CDD, for both C and N, the region of charge accumulation extends along the plane formed by these four Cr atoms. The 2D CDD analysis again revealed a significant charge increase between the C/N atom and the Cr side compared to the Co side, indicating stronger covalent bonding with Cr, similar to the results shown in Fig. 5(a). The fact that both C and N form stronger covalent bonds with Cr than with Co is consistent with our previous findings for Co–X binary alloys [44], which explains why the variation in charge for Cr in the 1NN shell was higher than that for the other elements, as shown in Fig. 3.

Fig. 6 presents the calculated versus predicted data from the multiple regression analysis of the relationship between E_{formX} across the 144 sites and the 1NN shell features.

Figs. 6(a) and (b) show the results obtained when the number of alloying atoms in the 1NN shell was used as the explanatory variable. We call the model as “alloying atom-count model”. In this model, the total number of alloying atoms in the 1NN shell is six. A multiple regression analysis was performed using the number of Co atoms as a reference. The regression equations are as follows:

$$E_{\text{formC,1NN}} (\text{eV}) = -0.048N_{\text{Cr}} + 0.189N_{\text{W}} + 0.075N_{\text{Ni}} + 0.263 \quad (3)$$

$$E_{\text{formN,1NN}} (\text{eV}) = -0.253N_{\text{Cr}} + 0.037N_{\text{W}} + 0.109N_{\text{Ni}} - 0.065 \quad (4)$$

where N_Y ($Y = \text{Cr}, \text{W}, \text{or Ni}$) represents the number of each element type in the 1NN shell. The adjusted R^2 values for these regression equations were 0.509 for C and 0.848 for N. For both C and N, the partial regression coefficient for N_{Cr} was the smallest (negative), indicating that a larger number of Cr atoms in the 1NN shell contributed to the stabilization of the C and N sites. This trend not only correlates with the strong Cr–C/N bonding shown in Fig. 5 but also aligns with the tendency observed in Co–X binary alloys [44]. Because the partial regression coefficients for N_{W} and N_{Ni} are positive, W and Ni are considered to destabilize C and N relative to Co. For N, the high adjusted R^2 value (> 0.8) indicates that the stable octahedral sites can be explained by the elemental affinity within the 1NN shell. Conversely, for C, although a correlation was identified (adjusted $R^2 > 0.5$), it was notably lower than that for N.

Figs. 6(c) and (d) show the results obtained when the types of bonds between the alloying atoms in the 1NN shell were used as explanatory variables. Again, we call the model as “alloying bond model”. This model, the total number of alloying bonds in the 1NN shell is 12. A multiple regression analysis was performed using the number of Co–Co bonds as a reference. The regression equations are as follows:

$$\begin{aligned} E_{\text{formC,1NN-1NN}} (\text{eV}) = & 0.003N_{\text{Co-Cr}} + 0.088N_{\text{Co-W}} + 0.019N_{\text{Co-Ni}} \\ & - 0.035N_{\text{Cr-Cr}} - 0.042N_{\text{Cr-W}} + 0.034N_{\text{Cr-Ni}} - 0.039N_{\text{W-W}} \\ & + 0.102N_{\text{W-Ni}} + 0.048N_{\text{Ni-Ni}} + 0.186 \end{aligned} \quad (5)$$

$$\begin{aligned} E_{\text{formN,1NN-1NN}} (\text{eV}) = & -0.059N_{\text{Co-Cr}} + 0.035N_{\text{Co-W}} + 0.027N_{\text{Co-Ni}} \\ & - 0.117N_{\text{Cr-Cr}} - 0.108N_{\text{Cr-W}} - 0.027N_{\text{Cr-Ni}} - 0.149N_{\text{W-W}} \\ & + 0.086N_{\text{W-Ni}} + 0.061N_{\text{Ni-Ni}} - 0.101 \end{aligned} \quad (6)$$

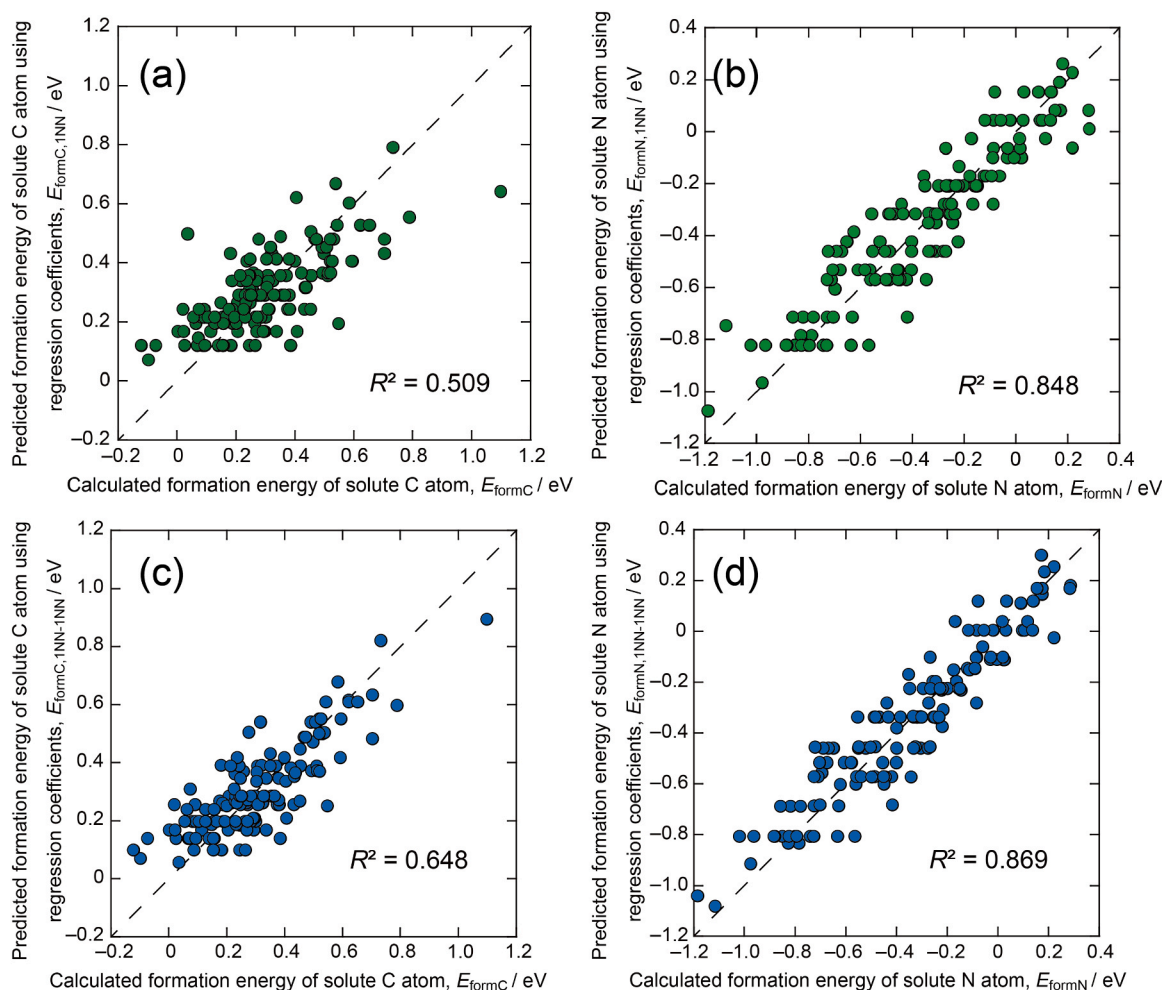


Fig. 6. Comparison between the calculated and predicted formation energies of solute C/N using multiple regression analysis. The predictions for (a) C and (b) N were derived from the number of each alloying atom in the 1NN shell (alloying atom-count model), whereas those for (c) C and (d) N were derived from the types of interatomic bonds within the 1NN shell (alloying bond model).

where N_Z ($Z = \text{Co-Cr}, \text{Co-W}, \text{Co-Ni}, \text{Cr-Cr}, \text{Cr-W}, \text{Cr-Ni}, \text{W-W}, \text{W-Ni}$, or Ni-Ni) represents the number of alloying bonds between the alloying atoms in the 1NN shell. The adjusted R^2 values for C and N were 0.648 and 0.869, respectively. In this model, the partial regression coefficients for terms involving Cr ($N_{\text{Co-Cr}}, N_{\text{Cr-Cr}}, N_{\text{Cr-W}},$ and $N_{\text{Cr-Ni}}$) tended to be low for both C and N. This is consistent with the alloying atom-count model, in which a larger number of Cr atoms in the 1NN shell contributes to site stability. An interesting behavior was observed for W by comparing the two regression models. In terms of the number of alloying atom alone, W destabilized the sites for both C and N. However, the partial regression coefficient for $N_{\text{W-W}}$ exhibited a low (negative) value for both C and N. Although the statistical reliability of this specific result is limited, as there are only two W-W pairs among the 144 octahedral sites, this suggests that W may also contribute to C and N stabilization depending on its specific local atomic configuration.

The adjusted R^2 values for this model increased for both C and N compared with the alloying atom-count model, highlighting the importance of considering the specific geometric arrangement of alloying atoms in the 1NN shell. For example, the 3Co-3Cr-fac (the most stable site for C) and 3Co-3Cr-mer configurations were identical in terms of the alloying atom-count model. However, their alloying bond configurations differed; 3Co-3Cr-fac had $N_{\text{Co-Cr}} = 6$ and $N_{\text{Cr-Cr}} = 3$, whereas 3Co-3Cr-mer had $N_{\text{Co-Cr}} = 8$ and $N_{\text{Cr-Cr}} = 2$. Substituting these values into Eq. (5) yields predicted $E_{\text{formC},1\text{NN}-1\text{NN}}$ values of 0.07 eV for 3Co-3Cr-fac and 0.14 eV for 3Co-3Cr-mer, whereas the actual DFT-

calculated E_{formC} values were -0.12 and 0.07 eV, respectively. Thus, the alloying bond model successfully captured the physical reality that 3Co-3Cr-fac is more stable than 3Co-3Cr-mer, a distinction that is impossible to identify using the alloying atom-count model alone. However, the adjusted R^2 value for C remained modest, leaving approximately 35% of the variance in E_{formC} unexplained. The relatively low R^2 value for C limits predictive performance. This difference in prediction accuracy between C and N may be interpreted in terms of charge variation in the 1NN shell (Fig. 3). For N, the value for Cr in the 1NN shell is significantly higher, indicating the formation of strong covalent bonds. In contrast, for C, although the charge variation for Cr is higher than for Co and Ni, the differences among the elements are not as pronounced as those observed for N. Because C exhibits smaller element-dependent differences in charge variation, resulting in relatively small variation in covalent bond strength, the stability of C is considered more susceptible to complex geometric configurations within the 1NN shell or to atomic arrangements extending to the 2NN shell and beyond. Elucidating the intrinsic mechanisms underlying these extended effects will be a subject of future work.

Regardless of the regression model, it is evident that Cr in the 1NN shell exerts a more profound influence on the stability of C and N than any other alloying element. Fig. 7 shows the relationship between the number of Cr atoms in the 1NN shell and E_{formX} . Consistent with the regression analysis, E_{formX} decreases as the number of Cr atoms increases for both C and N. The trend indicated by the regression line slope was

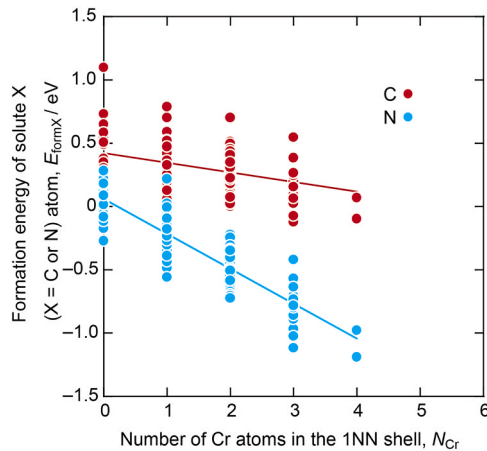


Fig. 7. Effect of the number of Cr atoms in the 1NN shell on the formation energy of the solute C/N.

more pronounced for N than for C. In this context, although there are no reports of short-range order (SRO) formation for C in CoCrNi alloys, the formation of Cr–N SRO has been reported with N addition [60]. The strong dependence of N stability on the 1NN Cr atoms observed in this study suggests a high probability of Cr–N SRO formation in the CCWN quaternary alloy.

3.3. Effect of C/N addition on the plastic deformation mechanism

Fig. 8 shows the average GSFE curves for the CCWN-without, CCWN-C, and CCWN-N models.

The CCWN-without curve is the average of two GSFE curves, whereas the CCWN-C and CCWN-N curves are the averages of 32 GSFE curves. The individual GSFE curves for each octahedral site are shown in Fig. S4. Compared to CCWN-without, the overall GSFE values increased with the C/N addition. This indicates an increased resistance to partial dislocation emission on the (111) plane containing C/N atoms in the CCWN quaternary alloys. Table 2 summarizes the corresponding changes in the GSFE parameters: $\Delta\gamma_{USF}$, $\Delta\gamma_{ISF}$, $\Delta\gamma_{UTF}$, and $\Delta\gamma_{ESF}$. $\Delta\gamma_{ISF}$ was 65 ± 40 and 45 ± 46 $\text{mJ}\cdot\text{m}^{-2}$ for C and N addition, respectively.

These results demonstrate that both C and N act as SFE-increasing elements in the CCWN quaternary alloy. Because both C and N increase $\Delta\gamma_{ISF}$, their addition suppresses SIMT as a plastic deformation mechanism. This aligns with our previous findings that C/N addition

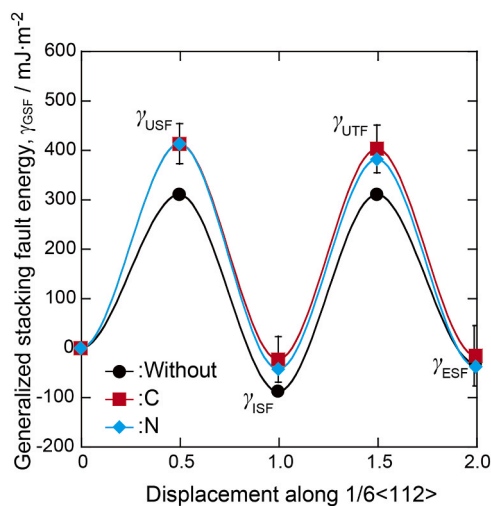


Fig. 8. Average GSFE curves of the CCWN-without, CCWN-C, and CCWN-N models.

Table 2

Changes in GSFE and twinnability with C/N addition.

	$\Delta\gamma_{USF} / \text{mJ}\cdot\text{m}^{-2}$	$\Delta\gamma_{ISF} / \text{mJ}\cdot\text{m}^{-2}$	$\Delta\gamma_{UTF} / \text{mJ}\cdot\text{m}^{-2}$	$\Delta\gamma_{ESF} / \text{mJ}\cdot\text{m}^{-2}$	$\Delta\eta$
C	103 ± 31	65 ± 40	92 ± 40	16 ± 40	0.024 ± 0.102
N	103 ± 41	45 ± 46	71 ± 48	-6 ± 61	0.075 ± 0.123

increases $\Delta\gamma_{ISF}$ in Co–X binary alloys [44]. Although the average increase in $\Delta\gamma_{ISF}$ tends to be slightly higher for C than for N, the large standard deviations suggest no significant difference between the C and N. In a CoCrNi alloy, the $\Delta\gamma_{ISF}$ values induced by C and N additions are reported to be 54 $\text{mJ}\cdot\text{m}^{-2}$ and 58 $\text{mJ}\cdot\text{m}^{-2}$, respectively, using a direct shear deformation method with SQS and supercell models [61], an approach similar to the present calculations. These values are comparable to the $\Delta\gamma_{ISF}$ values of C and N obtained in our calculations, indicating that C and N exhibit similar behavior in $\Delta\gamma_{ISF}$ in both the CoCrNi alloy and the CCWN quaternary alloy. Experimentally, it has been reported that C addition to the CCWN quaternary alloy suppresses SIMT [47], which is in agreement with our present calculations.

Enhanced UTS and ductility are expected when deformation twinning is promoted as a plastic deformation mechanism. To compare the propensity for dislocation slip versus twinning in fcc metals, the intrinsic twinnability parameter η is commonly used [62], which is defined as:

$$\eta = \frac{\gamma_{USF} - \gamma_{ISF}}{\gamma_{UTF} - \gamma_{ISF}}. \quad (7)$$

Compared to other twinnability parameters [63,64], η evaluates intrinsic twinnability without assuming pre-existing microstructures such as crack tips or grain boundaries. A higher η value indicates a greater susceptibility to deformation twinning. For the CCWN-without, η was 1.007. Because this value is close to 1, the CCWN-without can be considered an alloy in which dislocation slip and deformation twinning occur to a similar extent. For the CCWN-C and CCWN-N models, η was 1.031 ± 0.102 and 1.082 ± 0.123 , respectively. The changes in η induced by C/N addition ($\Delta\eta$) are presented in Table 2. The positive $\Delta\eta$ values indicate a tendency for deformation twinning to be promoted upon C and N additions. However, it should be noted that the standard deviations for $\Delta\eta$ are considerably large relative to their mean values. This substantial scatter indicates that statistical significance should be interpreted cautiously and suggests that although the overall trend favors twinning, plastic deformation is strongly influenced by local atomic fluctuations and the specific environments surrounding the interstitial atoms. N addition to a CoCrFeNiMn alloy has been reported to result in a negative $\Delta\eta$ and to experimentally suppress deformation twinning [26]. This differs from the behavior of N addition observed in the present calculations. Since the CCWN quaternary alloy investigated in this study does not contain Fe or Mn, this suggests that the presence of Fe and Mn changes the effect of N on η .

3.4. Effects of C/N addition on the mechanical properties

In this section, we discuss the effects of C/N addition on the mechanical properties of the CCWN quaternary alloy based on the insights obtained in this study.

First, we examined the effect of C/N addition on the yield strength. For interstitial-element additions up to approximately 1 mol%, the change in the shear modulus is often negligible [13,14], and the degree of solid-solution strengthening primarily depends on the lattice distortion [65]. Because the increases in the lattice constant, namely, the macroscopic lattice distortions, induced by C and N addition, were comparable in this study, the increments in the yield strength due to solid-solution strengthening are considered to be similar for both C and N addition. By contrast, the formation of Cr–N SRO has been suggested

for N addition. To investigate the effect of Cr in the 1NN shell, analogous to Cr–N SRO, on the GSFE, we evaluated how the number of Cr atoms in the 1NN shell of the perfect crystal affects the GSFE for N. Fig. 9 shows the average GSFE for the CCWN-without and CCWN-N models, categorized according to whether the 1NN shell of the perfect crystal contains fewer than three Cr atoms or three or more.

The overall GSFE values for N increase when three or more Cr atoms are present, compared to fewer than three. This indicates that an abundance of Cr around N increases the resistance to partial dislocation emission on the (111) plane. Consequently, when Cr concentrates around N, in a manner similar to Cr–N SRO, it provides resistance to plastic deformation and is expected to contribute to an increase in the yield strength of the alloy. A detailed investigation of how explicit Cr–N SRO domains systematically alter the plastic deformation mechanisms, however, remains an important topic for future work. Notably, previous experimental studies have also reported that SRO arising from N addition contributes to an increase in yield strength. For example, in the $\text{Co}_{20}\text{Cr}_{20}\text{Fe}_{30}\text{Mn}_{24}\text{Ni}_6$ alloy [11], it has been reported that the addition of 1 mol% N leads to a further increase in yield strength (140 MPa) owing to SRO formation, in addition to an increase in solid-solution strengthening (62 MPa). Therefore, while the addition of both C and N to the CCWN quaternary alloy increases the yield strength via solid-solution strengthening, N addition is expected to cause a greater increase than C addition because of the supplementary strengthening effect of SRO formation.

Next, we discuss the effects of the C/N additions on the UTS and ductility. In conventional Co–Cr-based alloys [6,34,66], the formation of the ϵ -phase via SIMT has been reported to reduce ductility because the γ/ϵ phase boundaries act as crack initiation sites. Similarly, for the CCWN quaternary alloy [47], it has been reported that the addition of C suppresses SIMT, thereby enhancing ductility. In the present study, we demonstrated that both C and N addition increase γ_{ISF} and suppress SIMT. Consequently, N addition, similar to C addition, is expected to improve ductility.

Furthermore, it is widely known that deformation twinning induces the TWIP effect, resulting in high UTS and ductility [10,11,17,67]. We have also reported that the onset of deformation twinning leads to high UTS and ductility in a Co–Cr–Fe–Ni–Mo alloy [28]. In the present study, both C and N addition tended to promote deformation twinning. An experimental investigation of the relationship between C/N addition and twinnability in the CCWN quaternary alloy is currently underway.

Based on the above discussion, the addition of either C or N to the CCWN quaternary alloy is expected to lead to high UTS and ductility by

suppressing SIMT and promoting deformation twinning. However, a critical distinction arises regarding the yield strength. Specifically, if the goal is to enhance the overall strength for structural applications, N addition is highly effective because of the anticipated increase in the yield strength associated with SRO formation. Conversely, the present fundamental results suggest that C addition can promote the TWIP effect without causing an excessive increase in yield strength. These insights are expected to serve as a useful theoretical basis for future alloy design strategies targeting applications that require a concurrent combination of low yield strength, high UTS, and high ductility, such as balloon-expandable stents.

4. Summary

In this study, the stability of interstitial C/N atoms and their effects on the GSFEs in Co–Cr–W–Ni quaternary alloys were systematically investigated using first-principles calculations. C/N-added quaternary alloy models were constructed by combining SQS and supercell methods, where the stable octahedral sites for C/N were determined from an energetic perspective. GSFE analysis was performed by introducing direct shear deformation into the supercell, allowing the C/N atoms to migrate based on the single diffusion hop mechanism. The key insights obtained from this study are summarized as follows,

- Multiple regression analysis revealed that E_{formX} for both C and N correlate with the alloying atom-count and bond models in the 1NN shell. Notably, the presence of Cr predominantly contributes to the stabilization of both C and N in the octahedral sites.
- For N, the variation in E_{formN} can be largely explained by the alloying atom-count model in the 1NN shell. Because the stabilizing effect of Cr was significantly stronger for N than for C, the formation of Cr–N SRO is suggested.
- The overall GSFE curves increased with the addition of either C or N. The concomitant increase in γ_{ISF} indicates that SIMT is suppressed as a plastic deformation mechanism. Simultaneously, the increased twinnability demonstrates that C/N addition tends to promote deformation twinning.

Consequently, regarding the mechanical properties, the addition of either C or N to the CCWN quaternary alloy is expected to enhance ductility by suppressing SIMT and to offer a potential pathway toward excellent UTS and ductility properties through the promotion of deformation twinning. Compared with C addition, N addition is anticipated to lead to a more substantial increase in yield strength owing to the supplementary strengthening effect of SRO formation. Ultimately, these GSFE-based findings are intended to provide foundational data for the development of balloon-expandable stents; however, experimental validation will be required, which is the focus of our future work.

Declaration of Generative AI and AI-assisted technologies in the writing process

During the preparation of this manuscript, the authors used ChatGPT solely to translate the initial draft from Japanese to English. After using this tool, we carefully reviewed and edited the text and assumed full responsibility for the final content of the article.

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Declaration of Competing Interest

The authors declare that no commercial interests or relationships

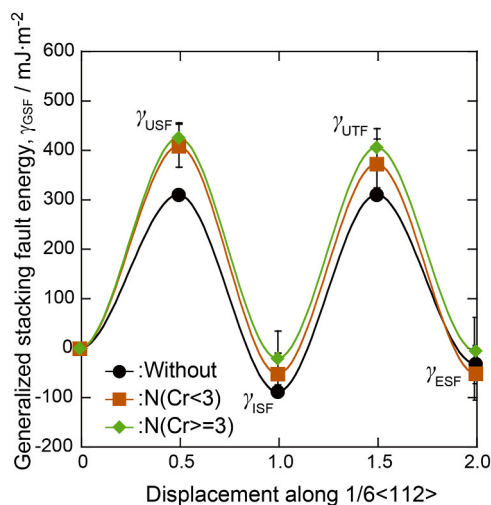


Fig. 9. Average GSFE of the CCWN-without model, alongside the CCWN-N models partitioned into two groups: those containing fewer than three, and those with three or more, Cr atoms in the 1NN shell of the perfect crystal.

have influenced this paper.

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Calculations were performed using a supercomputing system at the Institute for Materials Research (IMR), Tohoku University.

Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at [doi:10.1016/j.mtcomm.2026.115937](https://doi.org/10.1016/j.mtcomm.2026.115937).

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