Stacking fault energy of face-centered cubic metals: thermodynamic and \textit{ab initio} approaches

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Abstract

The formation energy of the interface between face-centered cubic (fcc) and hexagonal close packed (hcp) structures is a key parameter in determining the stacking fault energy (SFE) of fcc metals and alloys using thermodynamic calculations. It is often assumed that the contribution of the planar fault energy to the SFE has the same order of magnitude as the bulk part, and thus the lack of precise information about it can become the limiting factor in thermodynamic predictions. Here, we differentiate between the interfacial energy for the coherent fcc(1 1 1)/hcp(0 0 0 1) interface and the 'pseudo-interfacial energy' that enters the thermodynamic expression for the SFE. Using first-principles calculations, we determine the coherent and pseudo-interfacial energies for six elemental metals (Al, Ni, Cu, Ag, Pt, and Au) and three paramagnetic Fe–Cr–Ni alloys. Our results show that the two interfacial energies significantly differ from each other. We observe a strong chemistry dependence for both interfacial energies. The calculated pseudo-interfacial energies for the Fe–Cr–Ni steels agree well with the available literature data. We discuss the effects of strain on the description of planar faults via thermodynamic and \textit{ab initio} approaches.

Keywords: interfacial energy, stacking fault energy, \textit{ab initio}

(Some figures may appear in colour only in the online journal)

1. Introduction

In metals with face-centered cubic (fcc) structure, dislocations can dissociate into Shockley partial dislocations connected by a faulted ribbon. The most often observed fault is the intrinsic stacking fault (ISF). Assuming infinite separation between the two partials, an ideal ISF is obtained by removing a single close packed fcc (1 1 1) layer from the perfect fcc matrix. The stacking fault energy $\gamma$ (SFE) is the excess energy associated with the ISF. SFE has been recognized as


Figure 1. Stacking sequences and local structures for an hcp precipitate embedded in an fcc matrix. Panel (a): one stacking fault in the fcc matrix which produces two hcp layers (i = 1). Panel (b): i (i > 1) stacking faults on every other fcc(1 1 1) plane producing an hcp structure with 2i layers. Asterisks mark the critical layers that might belong to both hcp and fcc phases.

an important parameter in describing the mechanical properties of fcc metals and alloys. The equilibrium partial dislocation separation is due to a balance between the restorative force raised from the SFE and the repulsive elastic force of the partial dislocations. Thus, the SFE is of primary importance in many aspects of plasticity related to the dislocation mediated behaviors. In particular, the twinning induced plasticity (TWIP) mechanism has been associated with the size of the SFE. According to semi-empirical correlations [1], small SFE favors twinning, whereas large SFE leads to narrowly dissociated or undissociated dislocations and thus dislocation glide is favored. Very small or negative SFE is known to be responsible for the transformation induced plasticity (TRIP) mechanism.

The SFE is an intrinsic material property that can in principle be measured by carefully designed experiments. However, being a very small energy (usually of order of 10–100 mJ m$^{-2}$) an accurate determination is very difficult and the reported experimental data often carries very large error bars [2–4]. During the last decades several theoretical methods have been developed and employed for establishing reliable SFE databases. A very powerful method is based on the thermodynamic approach. In the model proposed by Olson and Cohen [5] (also referred as ‘volumetric model’), the stacking fault is treated as a two-layers embryo with the hexagonal close packed (hcp) structure embedded in the fcc matrix. Accordingly, the SFE of a laterally infinitely large stacking fault may formally be expressed as

$$\gamma = 2(F_{\text{hcp}}^{0} - F_{\text{fcc}}^{0})/A + 2\sigma^\ast,$$

(1)

where $F_{\text{hcp}}^{0}$ and $F_{\text{fcc}}^{0}$ are the equilibrium (indicated by the superscript $^{0}$) free energies per atom of the hcp and fcc phases, respectively, and A is the stacking fault area. Contemporary literature usually refers to $\sigma^\ast$ as the fcc/hcp interfacial energy and the $2\sigma^\ast$ term in equation (1) accounts for the two interfaces between the hcp embryo and the fcc matrix. This interfacial energy may, however, differ significantly from the coherent fcc/hcp interfacial energy ($\sigma^\ast$) since the hcp embryo in the above model of the stacking fault consists of only two layers, and the two fcc/hcp interfaces are likely to interact with each other. Additionally, in the thermodynamic calculations, the hcp phase is at equilibrium state, while in the coherent interface calculations, the hcp structure may have different volume and c/a ratio due to the coherency strain. Taking equation (1) as the definition of $\sigma^\ast$, all differences between the coherent stacking fault and the ‘embryo’ model are incorporated in the interfacial energy $\sigma^\ast$ [5]. Because of that in the following we refer to $\sigma^\ast$ as the pseudo-interfacial energy to distinguish it from the coherent interfacial energy $\sigma$ of fcc/hcp interface.

A throughout assessment of equation (1) can be found in [6].

No direct measurements of $\sigma^\ast$ are available. Instead, various efforts have been put forward to estimate $\sigma^\ast$ indirectly via equation (1) utilizing the measured SFE. For homogeneous Fe–Cr–Ni alloys, Olson and Cohen [5] using the calculated Gibbs free energies and the measured stacking fault energies [7] found $\sigma^\ast = 10–15$ mJ m$^{-2}$. Recently, Pierce et al [8] measured the chemical composition dependence of the SFE of Fe-Mn based alloys (Fe-22/25/28Mn-3Al-3Si wt.%) and calculated $\sigma^\ast$ according to equation (1) using the thermodynamic Gibbs energies. They showed that $\sigma^\ast$ ranges from 8 to 12 mJ m$^{-2}$ in Fe-Mn-Al-Si alloys and from 15 to 33 mJ m$^{-2}$ in binary Fe-Mn alloys. It was emphasized that $\sigma^\ast$ exhibits a strong dependence on the difference in Gibbs energies of the fcc and hcp phases. In particular, the Gibbs energy of the hcp phase, which has no precise description due to its thermodynamical instability, significantly influences the estimated $\sigma^\ast$ [9]. In practice, the pseudo-interfacial energy in thermodynamic calculations is often treated as an adjustable parameter to bring the theoretical SFE values in line with the observed deformation mechanisms [10]. Because of these difficulties, the predictive power of the thermodynamic SFE model is somewhat limited.

Ab initio quantum mechanical modeling is an alternative approach to determine the SFE. Recently, this approach was employed to study the SFE in transition metal alloys and stainless steels [11–14]. First-principles methods were also used to directly compute the coherent interfacial energies. Following the volumetric model, one can increase the thickness of the hcp layers (n = 2i; i is an integer) embedded in the fcc matrix, i = 1

8 In the original paper of Olson and Cohen [5], the SFE was expressed as

$$\gamma = n\rho_0(\Delta G^{\text{chem}} + E^{\text{str}}) + 2\sigma(n),$$

where $n\rho_0$ is the density of atoms in fcc (1 1 1) in moles per unit area, $\Delta G^{\text{chem}}$ and $E^{\text{str}}$ are the chemical free energy difference and strain energy defined as molar quantities. $n = 2$ for intrinsic stacking fault, $\sigma(n)$ is termed as interfacial energy and all differences between bulk and embryo properties are included in it. The interfacial energy is treated as a thickness dependent parameter, considering that the interfaces interact when $n$ is small. Notice that the experimentally measured SFE contains the coherent strain energy term, while it is typically not accounted for in thermodynamic SFE values. However, the coherency strain energy contribution decreases with increasing separation of the partial dislocations. It only matters at the early stage of dissociation. In the original work, the contribution of coherency strain energy was estimated to be less than 0.1 pct of the measured SFE and therefore neglected when calculating the interfacial energy of Fe–Cr–Ni alloys [5]. In the present work, the calculated SFE values correspond to infinitely large stacking faults and do not contain the strain energy contribution.
corresponds to one ISF, and \( i > 1 \) describes \( i \) stacking faults on every other (1 1 1) plane. Equivalently, they can be viewed as layered systems with two fcc/hcp interfaces separating the fcc and hcp parts. A similar model was recently adopted by Rosalie et al., when studying the fcc/hcp phase interface in Al-Ag-Cu alloys [15]. To first order, whether an atomic layer belongs to the fcc or the hcp phase depends on the stacking sequences of its two nearest neighboring layers. Namely, a layer having the two nearest neighbors with identical stacking sequence belongs to the hcp phase, otherwise it belongs to the fcc phase. This is illustrated schematically in figure 1. In panel (a), showing the situation for \( i = 1 \), we have marked the positions of the hcp/fcc interfaces when the system is considered as an hcp embryo embedded in the fcc phase; and the position of the stacking fault when the system is considered as an fcc phase with one stacking fault. At the interfaces there are critical layers (marked by asterisk) which might erroneously be considered as belonging to the hcp phase. However, these layers have two different nearest neighbor layers (corresponding to local fcc packing) and thus should not be taken as being energetically equivalent to the hcp layers [15]. Lee et al. recently calculated the interfacial energy of fcc Fe(1 1 1)/hcp Fe(0 0 0 1) using \textit{ab initio} methods [16]. They obtained an unreasonable interfacial energy (\( \sim 241 \text{ mJ m}^{-2} \)) compared to the commonly cited values (5–27 \text{ mJ m}^{-2}). However, carefully examining their interfacial structure, one finds that they placed the hcp/fcc interface at ‘...ABCABCABAB...’ instead of the correct position ‘...ABCABCA|BABAB...’. Therefore one fcc layer was erroneously taken as hcp layer, which resulted in the calculated ‘interfacial energy’ containing an additional term proportional to the energy difference between the fcc and hcp phases.

The above analysis is solely based on the stacking sequence from the structural point of view. There is no composition difference between the two sides of the interface. In cases where the composition of the precipitate deviates from that of the matrix, it may look straightforward to define the phase interface as the composition interface. However, the situation could be more complicated, such as in the case of the hcp/fcc interface in Al-Ag alloys. A recent study showed that for precipitates with thickness of 1–3 stacking faults, the thickness of the Ag-enriched region is considerably wider than the size of the hcp region indicating that the phase interface is more likely a structural interface in the Ag-enriched alloys. For precipitates with 6 stacking faults or more, the Ag-enriched zone was approximately equal to the width of the hcp region, indicating that the interface is a combination of structural and compositional interfaces [15].

In the present work, we study the coherent interfacial energies for fcc(1 1 1)/hcp(0 0 0 1) interfaces and the pseudo-interfacial energies in homogeneous metals and alloys. We employ an \textit{ab initio} total energy method that can account for alloying effects, so that the approach can easily be extended to solid solutions. Our mean-field approach avoids the ambiguous alloying configuration problem [17]. We notice, however, that in the case of segregation, occurring e.g. in the Al-Ag system, one should be careful when considering compositional and structural interfaces. Here we calculate the interface energies for pure fcc metals (Al, Ni, Cu, Ag, Pt and Au) and a few Fe–Cr–Ni alloys which represent the main building block of austenitic stainless steels. The coherent interfacial energy is calculated with respect to the number of hcp layers and the pseudo-interfacial energy is calculated according to the thermodynamic expression for SFE (equation (1)) using the calculated SFE values by the supercell model. We demonstrate that there is a significant difference between the coherent and the pseudo-interfacial energies. The large discrepancies originate from the actual definitions based on different reference structures. The rest of the paper is divided into two main sections. In section 2, we introduce the models used for calculating the interfacial energies and give the calculation details. The results are presented and discussed in section 3. The paper ends with conclusions.

2. Methodology

In the present work, we employ two methods for calculating the SFE and the interfacial energy of the fcc(1 1 1)/hcp(0 0 0 1) interface. The first method is based on a supercell model and provides a direct access to the interfacial energy as a function of layer thickness. It represents the most common method found in the literature to study the coherent interface. The second approach is the so-called axial interaction model (AIM), which maps the total energy into layer-layer interaction parameters offering a more straightforward insight into the mechanisms governing the interfacial energy in metals and alloys. This latter approach may easily be related to the thermodynamic model for calculating the SFE and thus provides a better understanding for the origin of the pseudo-interfacial energy.

2.1. Supercell model

To calculate the coherent interfacial energy, we build a series of supercells containing two fcc/hcp interfaces with various numbers of fcc (1 1 1) and hcp (0 0 0 1) layers. The supercells are denoted by \( m_{\text{fcc}} + nh_{\text{hcp}} \) or \( (m, n) \), where \( m \) and \( n \) are the numbers of fcc and hcp layers respectively. Periodic boundary conditions are applied. Considering the realistic situation that the lateral lattice constants are set up by the fcc matrix, the stacking fault layers and the hcp structure are distorted to form coherency with the fcc lattice. Hence, when there is a sizable difference between the equilibrium volumes of the fcc and hcp structures or the equilibrium hcp lattice has \( c_{\text{hcp}}/a_{\text{hcp}} \) far away from the ideal value (\( \sqrt{8/3} \)), the embedded hcp layers in the supercells will be distorted. In other words, the interlayer distance in the hcp part of the supercell will be different from the equilibrium \( \lambda_{\text{hcp}}^0 \) value. We therefore first relax the hcp structure with the constraint \( a_{\text{hcp}} = a_{\text{fcc}}^{111} = \sqrt{2}a_0 \) (\( a_0 \) being the fcc lattice parameter) to find the interlayer distance \( \lambda_{\text{hcp}} \). The interlayer distances for ‘bulk hcp’ inside the supercell (\( \lambda_{\text{hcp}} \)), except the topmost ones (\( \lambda_{\text{top}} \)) which are the closest to the fcc/hcp interface, are fixed to \( \lambda_{\text{hcp}} \). The interlayer distances...
between the fcc(1 1 1) layers are kept at their equilibrium values, \( \lambda_{\text{fcc}}^0 = \sqrt{3}/3a_0 \). The topmost hcp interlayer distance \( \lambda_{\text{hcp}}^{\text{topmost}} \) and the interface separation between the fcc and hcp parts of the supercell \( \lambda_{\text{fcc/hcp}} \) are relaxed (see below).

Using the total energy \( F_{\text{fcc/hcp}}(m,n) \) of the \( m \text{fcc} + n \text{hcp} \) supercell, the interfacial energy may be calculated as

\[
\sigma(m,n) = \frac{F_{\text{fcc/hcp}}(m,n) - mF_{\text{fcc}}^0 - nF_{\text{hcp}}^0}{2A},
\]

where \( F_{\text{fcc}}^0 \) is the equilibrium total energy of the fcc lattice (per atom), \( F_{\text{hcp}}^0 \) is the total energy of the constrained hcp lattice (per atom), which usually is larger than the actual equilibrium hcp energy \( F_{\text{hcp}}^0 \), \( A = \sqrt{3}/4a_0^2 \) is the area of the interface and the factor 2 stands for the two interfaces present in the supercell. For a large enough \( m \), the interfacial energy should converge with increasing \( n \) towards a constant value representing the coherent fcc/hcp phase interface energy \( \sigma \).

For \( n = 0 \), the interfacial energy \( \sigma(m,0) \) is obviously zero. For \( n = 2 \), the supercell has two hcp layers which can also be viewed as one intrinsic stacking fault (figure 1(a)). Hence, the intrinsic stacking fault energy may be computed from the present \((m,2)\) supercell energy as

\[
\gamma(m) = \frac{F_{\text{fcc/hcp}}(m,2) - (m+2)F_{\text{fcc}}^0}{A}.
\]

With increasing the fcc layer thickness \((m \to \infty)\) the above \( \gamma(m) \) converges to the true SFE.

In the present application, the number of fcc layers was chosen to be 9 \((m = 9)\) which was found to be large enough to remove the interaction due to the periodic boundary conditions and which leads to converged SFE values. The number of hcp layers, on the other hand, was increased from 0 to 8 with an increment of 2. The interfacial energy is usually a very small quantity and it is very sensitive to the numerical details used in the \( ab \) \textit{initio} calculations. In order to keep the numerical noises at minimum, the fcc energy \( F_{\text{fcc}}^0 \) was calculated from the energy of the \( 9\text{fcc} + 0\text{hcp} \) supercell as \( F_{\text{fcc}} = F_{\text{fcc/hcp}}(9,0)/9 \). The energy of the distorted hcp phase was evaluated from the difference between the total energies of the \((9,8)\) and \((9,6)\) supercells, \( F_{\text{hcp}}^0 = [F_{\text{fcc/hcp}}(9,8) - F_{\text{fcc/hcp}}(9,6)]/2 \). We notice that computing \( F_{\text{hcp}}^0 \) from the \((9,8)\) and \((9,4)\) supercells leads to very similar results as those presented here.

We studied the relaxation of the interface between the fcc and hcp parts of the supercell \( \lambda_{\text{fcc/hcp}} \) and found that the fully relaxed layer separation is very close to the average value of the interlayer separations of fcc(1 1 1) and hcp(0 0 0 1) layers. Therefore, in order to reduce the computational load, for all supercells we used \( \lambda_{\text{fcc/hcp}} \approx (\lambda_{\text{fcc}}^0 + \lambda_{\text{hcp}}^0)/2 \). The topmost hcp interlayer distance \( \lambda_{\text{hcp}}^{\text{topmost}} \) was always relaxed, which turns out to be important especially when \( n \) is small.

### 2.2. Axial interaction model

The SFE and the interfacial energy may be estimated using the axial interaction model (AIM) [13, 18, 19]. Within this model, along the [1 1 1] direction, a particular stacking sequence of the close-packed (1 1 1) planes can be mapped by a set of variables \( S_i \), where \( i \) is the layer index. \( S_i \) may take two possible values: +1 if the layer at site \((i+1)\) follows the ideal fcc stacking sequence, else a value of −1 is assigned. Thus, the energy of a structure with a particular stacking sequence can be expanded as

\[
F = J_0 - J_1 \sum_i S_i S_{i+1} - J_2 \sum_i S_i S_{i+2} - J_3 \sum_i S_i S_{i+3} + O(J_4),
\]

where the sums run over the atomic layers. \( J_0 \) is the energy per unit cell in one layer if the interactions between layers are disregarded. \( J_1, J_2 \ldots \) are the nearest-neighbor, next nearest-neighbor, etc, interaction parameters between layers. \( O(J_4) \) stands for the contribution from the higher order terms. Using this expression, the energies of an intrinsic stacking fault, hcp and double hexagonal close-packed (dhcp) structures relative to the fcc phase can be expressed as

\[
\begin{align*}
F_{\text{sf}}^0 - F_{\text{fcc}}^0 &= 4J_1 + 4J_2 + 4J_3 + O(J_4), \\
F_{\text{hcp}}^0 - F_{\text{fcc}}^0 &= 2J_1 + 2J_2 + O(J_4), \\
F_{\text{dhcp}}^0 - F_{\text{fcc}}^0 &= J_1 + J_2 + J_3 + O(J_4).
\end{align*}
\]

Here the superscript \( \delta \) expresses the fact that the corresponding energies are not the equilibrium values (all structural parameters are kept at the ideal fcc values). Keeping the interactions up to the third order in equation (5) (i.e. neglecting \( J_4 \) and all higher order terms), for the SFE we get

\[
\gamma^{(3)} = (F_{\text{hcp}}^\delta + 2F_{\text{dhcp}}^\delta - 3F_{\text{fcc}}^\delta)/A.
\]

This third order AIM expression was adopted by Vitos \textit{et al} [2, 11–13] in the case of paramagnetic steel alloys and it was found to lead to SFE values in good agreement with the experimental results. Truncating equation (5) after the first order (i.e. neglecting \( J_2 \) and all higher order terms), leads to

\[
\gamma^{(1)} = 2(F_{\text{hcp}}^\delta + F_{\text{fcc}}^\delta)/A,
\]

which is the lowest order approximation for the SFE in terms of interaction parameters.

It is important to realize that when the in-plane and out-of-plane lattice constants are fixed to those of the ideal fcc lattice, \( F_{\text{fcc}}^0 \) in equations (5)–(7) represents the equilibrium fcc total energy, but the other energies do not necessarily correspond to the equilibrium values for the respective structure. That is because equation (4) does not make a difference whether an interaction \( J_i \) is in the fcc, hcp or dhcp matrix. Because of that the AIM cannot account for layer relaxation or magnetic effects which may differ for different packing sequences. This is a shortcoming of the AIM and should be taken into consideration when comparing the AIM predictions with the direct
calculations using a supercell technique. In particular, $F_{\text{hcp}}^p$ in equations (5)–(7) represents the total energy of an hcp lattice with $a_{\text{hcp}} = \sqrt{2}/2a_0$ and ideal interlayer distance $\lambda_{\text{hcp}} = \lambda_{\text{fcc}}^0$ (meaning an hcp lattice with $c_{\text{hcp}} = \sqrt{8}/3$).

We recall that in equation (1), the SFE is expressed as twice the free energy difference between the equilibrium hcp and fcc phases plus twice the pseudo-interfacial energy $\sigma^*$. Thus using equation (7), we arrive at

$$\gamma = \gamma^{(1)} - 2\delta/a + 2\sigma^*.$$  

(8)

Here $\gamma^{(1)} = 2\delta/a = 2(F_{\text{hcp}}^0 - F_{\text{fcc}}^0)/a$ may be taken as the SFE without fcc/hcp interface energy correction. The correction term in equation (8) is defined as $\delta \equiv F_{\text{hcp}}^e - F_{\text{hcp}}^0$.

From equations (6) and (8) we infer that when $\delta$ is small, the pseudo-interfacial energy is in fact a correction term to $\gamma^{(1)}$ due to the second and higher order layer interactions. This situation can happen when the equilibrium hcp lattice has the same volume as the fcc lattice and ideal hexagonal axial ratio.

Using the AIM, one may establish a simple relation based on the structural energy differences in equation (5) that can be used to estimate the pseudo-interfacial energy. Approximating the true SFE energy by $\gamma^{(3)}$, from equations (6) and (7) we get

$$\sigma^{(3)} = (2F_{\text{dhp}}^s - F_{\text{hcp}}^e - F_{\text{hcp}}^0)/(2A) + 2\delta/a.$$  

(9)

This expression includes interlayer interactions up to the third order ($J_3$). We notice that for most of the metals $F_{\text{dhp}}^s$ is close to the equilibrium dhcp energy $F_{\text{dhp}}^0$. Using the first term in the right hand side of equation (9), we may define $\bar{\sigma}^{(3)} = \sigma^{(3)} - 2\delta/a$. This quantity may be considered a reasonable approximation to the pseudo-interfacial energy in equation (1) when $\delta$ is negligible.

2.3. Total energy method

The total energies were calculated using the exact muffin-tin orbitals (EMTO) method [20, 21] in combination with the coherent potential approximation (CPA) [22, 23]. The EMTO-CPA approach is an appropriate tool for describing systems with chemical disorder. Spin-polarized calculations were performed for Ni. In the self-consistent calculations, the one-electron equations were solved within the scalar-relativistic approximation and soft-core scheme. However, for the three Fe–Cr–Ni alloys, we adopted the frozen-core scheme in order to be able to compare the present results with previous theoretical values [11]. The Green function for the valence states was calculated for 16 complex energy points. In the muffin-tin basis set we included s, p, d and f orbitals. The k-point mesh was carefully tested and we used 1000–2000 uniformly distributed k-points in the irreducible wedge of the Brillouin zone for fcc, hcp and dhcp structures, and 363 k-points for the supercells. With these numerical parameters, the interfacial energy converges within an error of ~1 mJ m$^{-2}$. For the exchange-correlation functional the generalized gradient approximation of Perdew, Burke, and Ernzerhof was employed. The paramagnetic state of Fe–Cr–Ni alloys were modeled within the disordered local magnetic moment picture [24]. All calculations were performed at static (0 K) conditions.

### 3. Results and discussions

#### 3.1. Interfacial and stacking fault energies of fcc metals

Using the present total energy method, first we calculated the equilibrium lattice constants of six fcc metals: Al, Ni, Cu, Ag, Pt, and Au. For each system, the total energies were computed for five volumes around the expected equilibrium value and a Morse type of function [25] was fitted to extract the equilibrium lattice constant. Results are listed in table 1 together with former theoretical [26] and experimental values [27]. The present predictions are in excellent agreement with previous theoretical values and they are also close to the experimental data.

In table 1, we compare the equilibrium distances between the (1 1 1) layers for the fcc lattice ($\lambda_{\text{fcc}}^0$) and those between the (0 0 0 1) layers for the hcp lattice ($\lambda_{\text{hcp}}$). These hcp lattices are relaxed by constraining the in-plane lattice parameters to those of the fcc lattices, i.e. $a_{\text{hcp}} = \sqrt{2}/2a_0$. For each monatomic metal considered here, the equilibrium atomic volume of the fully relaxed hcp lattice is slightly larger than the fcc equilibrium volume and the corresponding equilibrium lattice constant is larger than the ideal value, i.e. $\lambda_{\text{hcp}} > \lambda_{\text{fcc}}^0$ (table 1). In the following, all supercells for interfacial energy calculations are built using the lattice parameters from table 1, (see section 2.1).

| Lattice parameter | Al | Ni | Cu | Ag | Pt | Au |
|-------------------|----|----|----|----|----|----|
| $a_0$             | 4.045 | 3.526 | 3.638 | 4.164 | 3.987 | 4.177 |
| $a_0$-Cal.$^a$    | 4.046 | 3.518 | 3.631 | 4.148 | 3.980 | 4.164 |
| $a_0$-Expt.$^b$   | 4.05 | 3.52 | 3.61 | 4.09 | 3.92 | 4.08 |
| $\lambda_{\text{hcp}}^0$ | 2.336 | 2.037 | 2.101 | 2.405 | 2.303 | 2.412 |
| $\lambda_{\text{hcp}}$ | 2.368 | 2.051 | 2.113 | 2.422 | 2.347 | 2.439 |
| $\delta_{\text{hcp}}$ | 2.850 | 2.489 | 2.566 | 2.936 | 2.789 | 2.931 |
| $\delta_{\text{dhp}}$ | 1.651 | 1.642 | 1.645 | 1.647 | 1.688 | 1.671 |

$^a$ [26]  
$^b$ [27]
are surprisingly large. For all metals in table 2, the 
\[ \sigma(9, n) \] obtained for Ag and Ni is

\[ \sigma(9, 4) = -21.7 (13) \]
\[ \sigma(9, 6) = -21.8 (12.7) \]
\[ \sigma(9, 8) = -21.8 (12.7) \]

The absolute value of the relative difference between the in-plane lattice parameters around 0.05%. It means that for these metals the hcp slab in the (9, n) supercells is only weakly deformed relative to the equilibrium hcp lattice. This is reflected in the very small values of \( F_{\text{hcp}}^{\Sigma} - F_{\text{hcp}} \) obtained for Ag and Ni \((\leq 50 \mu \text{Ry})\). For Ag, the interfacial energy is close to zero but for Ni we have \( \sigma(9, 8) \approx -8 \text{ mJ m}^{-2} \). In this respect, one may rule out the correlation between the size of the lattice strain at the coherent fcc(1 1 1)/hcp(0 0 0 1) interface and the size of the interfacial energy. On the other hand, the large variation of \( \sigma(9, n) \) as we scan the present simple metal (Al), the 3 \( \text{d} \) (Ni, Cu), 4 \( \text{d} \) (Ag) and 5 \( \text{d} \) (Pt, Au) transition metals indicates the importance of the chemistry around the planar fault.

In order to verify the present predictions for the interfacial energy, we carried out a set of independent supercell calculations for Al and Cu using the projector augmented wave (PAW) method [28, 29] as implemented in the Vienna ab initio simulation package (VASP) [30, 31]. In these additional calculations, the generalized gradient approximation (GGA) was considered to describe the exchange-correlation term [32]. The energy cut-off for the plane basis expansion was set to 600 eV for both metals, 45 \( \times 45 \times 5 \) k-point mesh with the Monkhorst–Pack scheme [33] was used to sample the Brillouin zone of the (9, n) supercell (corresponding to 914 k-points in the irreducible zone). We notice that the above k-mesh in VASP calculations ensured the same level of convergence as obtained in EMTO calculations. The structural relaxations, considering atomic positions and the length of the c-axis with fixed lateral lattice constant, were performed with the Methfessel–Paxton smearing method [34] with 0.2 eV smearing width. The maximum residual force is less than \( 10^{-3} \text{ eV Å}^{-1} \). Finally, the total energy for given structure was obtained by the tetrahedron method [35]. Since interfacial energies are very small, we calculated the total energy with \( 10^{-5} \text{ eV atom}^{-1} \) precision.

The theoretical equilibrium lattice constants for fcc Al and Cu from the VASP calculations are 4.040 and 3.635 Å, which are in good agreement with the present EMTO results. We computed the interfacial energies according to equation (2), with \( m = 9 \) and various \( n \). The interfacial energies for Al and Cu calculated with VASP are listed side by side with the EMTO results in table 2. Both of the two \emph{ab initio} methods give large negative interfacial energies for Al and nearly zero for Cu. We see a larger difference between the interfacial energies for Al obtained with the two methods \((-9 \text{ mJ m}^{-2})\) than for Cu. The larger error can be reduced by increasing the size of the supercell in the VASP calculations, for example, increasing fcc (1 1 1) layers to 12 leads to \( \sigma(12, 8) \approx -20 \text{ mJ m}^{-2} \). It seems that the VASP interfacial energy for Al converges slower, which is probably because that in the VASP calculations, the inter-layer distances are fully relaxed, compared to the local relaxations performed in the EMTO calculations. The general agreement between these two sets of data reflects the reliability of the present approach.

Next we turn to the SFE and the pseudo-interfacial energy. The present (9, 2) supercells are used in connection with equation (3) to find the SFE of the present fcc metals. The results are collected in table 3. Our \( \gamma \) values are in good agreement with the previous theoretical results [36, 38] and also with the limited number of experimental data [39, 41–45]. When comparing the theoretical and experimental SFE values one should keep in mind that the experimental data were obtained at room temperature whereas the theoretical values refer to 0 K neglecting all thermal contributions. The present \( \gamma \) values are used to derive the pseudo-interfacial energies. Using the equilibrium hcp \( F_{\text{hcp}}^{\Sigma} \) and fcc \( F_{\text{fcc}}^{\Sigma} \) total energies, we computed \( \gamma_{0}^{(1)} = \gamma_{0}^{(1)}(\text{fcc})/A \).

\[
\gamma_{0}^{(1)} = 2(F_{\text{hcp}}^{\Sigma} - F_{\text{fcc}}^{\Sigma})/A.
\]

We recall that \( \gamma_{0}^{(1)} \) is the first term in the right hand side of equation (1) so that the difference between \( \gamma \) and \( \gamma_{0}^{(1)} \) gives twice the pseudo-interfacial energy \( \sigma \). These results are also listed in table 3. We find that \( \sigma \) is almost zero for Cu and Ag, and intermediate for Ni and Au. The \( \sigma \) values for Al and Pt are the largest (in absolute value) among the present metals and both of them are negative. It is important to observe that except for Cu and Ag, the present \( \sigma \) values differ significantly from the \( \sigma(9, n) \) values listed in table 2. As we will show it in section 3.3., the main reason for the difference is the lattice constraint at the fcc (1 1 1)/hcp(0 0 0 1) interface which increases the reference hcp total energy \( F_{\text{hcp}}^{\Sigma} \) substantially relative to the equilibrium hcp energy \( F_{\text{hcp}}^{\Sigma} \).

| Table 2. Interfacial energies \( \sigma(9, n) \) (in mJ m\(^{-2}\)) for selected fcc metals as a function of the number of hcp layers \( n \) used in the supercell calculations. |
| --- |
| Al | Ni | Cu | Ag | Pt | Au |
| \( \sigma(9, 2) \) | \(-19.4 (13.8)\) | \(-4.4\) | \(-1.3 (0.2)\) | \(0.0\) | \(-24.1 \) | \(-0.8\) |
| \( \sigma(9, 4) \) | \(-21.7 (13.3)\) | \(-6.7\) | \(-0.6 (1.3)\) | \(-0.4\) | \(-24.4 \) | \(-1.6\) |
| \( \sigma(9, 6) \) | \(-21.8 (12.7)\) | \(-8.0\) | \(-0.3 (1.3)\) | \(-0.6\) | \(-24.8 \) | \(-1.8\) |
| \( \sigma(9, 8) \) | \(-21.8 (12.7)\) | \(-8.0\) | \(-0.3 (1.3)\) | \(-0.6\) | \(-24.8 \) | \(-1.8\) |

Note: The VASP results for Al and Cu are listed in parentheses. The error bar is estimated to be \( \pm 0.5 \text{ mJ m}^{-2} \).
would remove the difference between $\sigma'$ and $\sigma(9,n)$. However, associating $(F_{\text{hcp}}^{\text{SC}} - F_{\text{hcp}}^{\text{0}})$ merely to lattice strain given by the coherent interface could be misleading since $F_{\text{hcp}}^{\text{SC}}$ as extracted here from the supercell energies may contain additional terms due to the finite size effects (e.g. interaction between consecutive fcc/hcp interfaces).

For reference, in table 3, we also list results obtained using the AIM introduced in section 2.2. Comparing to the supercell results, the first order AIM ($\gamma^{(1)}$) gives acceptable SFE values for Ni, Cu, Ag and Au (within ~5% error), but strongly overestimates those for Al and Pt (by more than ~15%). The third order AIM ($\gamma^{(3)}$) somewhat improves the SFE results, especially for Al, but $\gamma^{(3)}$) for Pt still remains 33.5 mJ m$^{-2}$ (corresponding approximately to 11% error). To reach better agreement for Pt, one may need to keep more terms in equation (5) since a previous ab initio study indicated that the stacking fault in Pt induces a longer perturbation in the electronic structures than in other elemental metals [46].

Sticking to the 3rd order AIM approximation, one can use equation (9) to estimate the pseudo-interfacial energy $\sigma^{(3)}$. The accuracy of this approximation should be quite high when $\gamma^{(3)} \approx \gamma$. Indeed, the quoted figures in table 3 represent a reasonable approximation for most of the metals considered here: the differences between $\sigma^{(3)}$ and $\sigma^*$ being close to the errors of the calculations. Exception is Pt, for which $\sigma^{(3)}$ is surprisingly far from the ‘true’ $\sigma^*$ value. This is due to the fact that for Pt the 3rd order AIM fails to reproduce the SFE of the supercell model. In table 3, we also present the AIM estimates for the interfacial energy by excluding the lattice distortion effect (i.e. dropping the $2\delta A$ term in equation (9)). The reason for testing such simplified formula is that within the 3rd order AIM approximation we have $\sigma^{(3)} - 2\delta A = 2J_2A$, i.e. the interfacial energy is given by the second order nearest-neighbor layer interaction parameter $J_2$. For most of the metals $2J_2A$ gives a plausible estimate for the interfacial energy. However, for Au, where the 3rd order

### Table 3. Theoretical intrinsic SFE ($\gamma$) and pseudo-interfacial energies ($\sigma^*$) for selected fcc metals (in boldface).

|   | Al  | Ni  | Cu  | Ag  | Pt  | Au  |
|---|-----|-----|-----|-----|-----|-----|
| $\gamma$ | 117.5 | 153.6 | 47.5 | 17.3 | 308.0 | 32.7 |
| $\gamma^{(1)}$ | 139.3 (136.7) | 160.2 (159.2) | 50.4 (49.8) | 17.9 (17.1) | 359.1 (334.9) | 34.2 (30.7) |
| $\gamma^{(2)}$ | 135.5 | 156.9 | 48.6 | 15.8 | 319.8 | 25.2 |
| $\gamma^{(3)}$ | 123.5 (122.1) | 158.1 (157.4) | 50.7 (50.5) | 18.4 (18.1) | 341.5 (324.7) | 32.7 (30.5) |
| Theory | 107$^{a}$, 130$^{b}$ | 153$^{a}$, 110$^{b}$ | 47$^{a}$, 41$^{b}$, 56$^{c}$ | 17$^{a}$, 18$^{b}$, 34$^{c}$ | 310$^{a}$, 324$^{b}$, 393$^{c}$ | 31$^{a}$, 33$^{b}$, 59$^{b}$ |
| Expt. | 166$^{d}$, 120$^{e}$ | 125$^{f}$ | 55$^{e}$, 41$^{b}$ | 22$^{g}$, 16$^{i}$ | 322$^{f}$ | 50$^{f}$, 32$^{i}$ |
| $\sigma^*$ | −9.0 | −1.7 | −0.6 | 0.7 | −5.9 | 3.7 |
| $\sigma^{(3)}$ | −6.0 (−6.7) | 0.6 (0.2) | 1.0 (0.9) | 1.3 (1.1) | 10.8 (2.4) | 3.8 (2.6) |

### Table 4. Lattice parameters of the fcc and hcp structures for three selected Fe$_{100-x-y}$Cr$_x$Ni$_y$ alloys.

| Lattice parameter | Fe$_{68}$Cr$_{12}$Ni$_{20}$ | Fe$_{56.5}$Cr$_{13.5}$Ni$_{20}$ | Fe$_{70.5}$Cr$_{13.5}$Ni$_{16}$ |
|------------------|--------------------------|-----------------------------|-----------------------------|
| $a_o$ | 3.606 | 3.606 | 3.605 |
| $a_o$-Cal. | 3.599$^a$ | 3.599$^b$ | 3.596$^c$ |
| $\lambda_{\text{hcp}}$ | 2.082 | 2.082 | 2.081 |
| $\lambda_{\text{fcc}}$ | 2.056 | 2.056 | 2.056 |
| $\delta_{\text{hcp}}$ | 2.556 | 2.555 | 2.555 |
| $\delta_{\text{hcp}}/\delta_{\text{hcp}}$ | 1.621 | 1.623 | 1.622 |
| $\lambda_{\text{hcp}}$ | 2.072 | 2.073 | 2.072 |

$^a$For Fe$_{68}$Cr$_{12}$Ni$_{20}$ [47].
$^b$For Fe$_{56.5}$Cr$_{13.5}$Ni$_{20}$ [47].
$^c$For Fe$_{70.5}$Cr$_{13.5}$Ni$_{16}$ [47].

Note: For the notations and units, see caption for table 1.

AIM is accurate, neglecting $2\delta A$ in equation (9) worsens the agreement between $\sigma^{(3)}$ and $\sigma^*$.

Before turning to the steel alloys, we briefly discuss a commonly used approximation within the AIM. In applications, the AIM is often used in connection with hcp and dhcp structural energies obtained for lattices constrained within the (000 1) plane but relaxed along the (1 1 1) direction [11, 13]. We refer to this scheme as the relaxed AIM (r-AIM) approximation. Notice that similar hcp structures are used here to build the inner part of the hcp slab within the $(m,n)$ supercells. To test this scheme for the present systems, in table 3 we list the SFE and interfacial energies obtained within the r-AIM approximation (numbers in parentheses). Since lattice relaxation lowers the hcp and dhcp energies, the corresponding SFE also become smaller in parentheses. Therefore, for Au, the 3rd order
Table 5. Interfacial energies $\sigma(9, n)$ (in mJ m$^{-2}$) for three selected Fe$_{100-x-y}$Cr$_x$Ni$_y$ alloys as a function of the number of hcp layers ($n$) used in the supercell calculations.

| Fe$_{66.5}$Cr$_{20}$Ni$_{13.5}$ | Fe$_{66.5}$Cr$_{13.5}$Ni$_{20}$ | Fe$_{70.5}$Cr$_{13.5}$Ni$_{16}$ |
|-----------------------------|-----------------------------|-----------------------------|
| $\sigma(9, 2)$              | 1.0                         | 0.5                         | 0.7 |
| $\sigma(9, 4)$              | $-0.9$                      | $-1.6$                      | $-1.7$ |
| $\sigma(9, 6)$              | $-2.1$                      | $-2.5$                      | $-3.0$ |
| $\sigma(9, 8)$              | $-2.1$                      | $-2.5$                      | $-3.0$ |

Note: The error bar is estimated to be $\pm 0.5$ mJ m$^{-2}$.

Table 6. Theoretical intrinsic SFE ($\gamma$) and pseudo-interfacial energies ($\sigma^*$) for selected Fe$_{100-x-y}$Cr$_x$Ni$_y$ alloys.

| Fe$_{66.5}$Cr$_{20}$Ni$_{13.5}$ | Fe$_{66.5}$Cr$_{13.5}$Ni$_{20}$ | Fe$_{70.5}$Cr$_{13.5}$Ni$_{16}$ |
|-----------------------------|-----------------------------|-----------------------------|
| $\gamma$                    | 30.6                        | 39.4                        | 38.2 |
| $\gamma^{0(1)}$             | 21.7 (15.2)                 | 30.3 (25.3)                 | 28.9 (23.1) |
| $\gamma^{0(2)}$             | 15.0                        | 22.8                        | 20.6 |
| $\gamma^{3(3)}$             | 28.9 (26.0)                 | 37.5 (35.0)                 | 36.0 (33.0) |
| Theory                      | 35$^a$                      | 50$^a$                      | 45$^a$ |
| Expt.                       | 32$^c$, 38$^b$, 41$^c$      | 46$^c$                      | 38$^c$ |
| $\sigma^*$                  | 7.8                         | 8.3                         | 8.8 |
| $\sigma^*^{(3)}$            | 7.0 (5.5)                   | 7.3 (6.1)                   | 7.7 (6.2) |
| $\delta^{(3)}$              | 3.7 (5.1)                   | 3.6 (4.8)                   | 3.5 (5.0) |

$^a$ [48], $^b$ [49].

$^c$ According to SFE $= 16.7 \pm 2.1\text{Ni-0.9Cr + }26\text{C} (\text{mJ m}^{-2})$ from [50].

$^d$ [12, 13].

Note: For notations see caption of table 3. The error bar is estimated to be $\pm 0.5$ mJ m$^{-2}$.

3.2. Interfacial and stacking fault energies of Fe$_{100-x-y}$Cr$_x$Ni$_y$ alloys

In this section, we apply the above developed and tested model to three Fe$_{100-x-y}$Cr$_x$Ni$_y$ alloys. We start from a 20% Cr and 20%Ni bearing ternary alloy and then first lower the amount of Cr to 13.5% and then the amount of Ni to 16%. By that, we can differentiate between the alloying effect of Cr and Ni on the SFE and interfacial energy of Fe–Cr–Ni alloy. We emphasize that the present results are obtained at 0 K, one should be careful when comparing with the experimental values measured at room temperature.

First we computed the equilibrium lattice parameter and equilibrium interlayer distance for thefcc and constrained hcp structures, respectively. The results are collected in table 4. We find that within the present approximation, the effects of Cr and Ni on the equilibrium lattice parameters of fcc and hcp structures are negligible. For these alloys, the equilibrium atomic volume of the fully relaxed hcp lattice is slightly smaller than that of fcc and the corresponding equilibrium $c_{\text{hcp}}/d_{\text{hcp}}$ ($c_{\text{hcp}}/d_{\text{hcp}}(001)$) is also smaller than $\sqrt[3]{8}$. Hence, when matching coherently the hcp(0 0 0 1) facet to fcc(1 1 1) facet, the layer-relaxed distorted hcp lattice should have smaller inter layer separation as compared to the ideal value, i.e., $\lambda_{\text{hcp}} < \lambda_{\text{fcc}}$ (table 4).

The calculated interfacial energies $\sigma(9, n)$ for the three Fe–Cr–Ni alloys are listed in table 5. Similarly to the mono-atomic systems, the variations of $\sigma(9, n)$ with increasing number of hcp layers are of the order of our numerical errors. For all three alloys, the converged interfacial energies are small and negative, with absolute values slightly larger than the present error bars. Considering $\sigma(9, n)$ with $n \geq 4$, one may conclude that both Cr and Ni addition to Fe–Cr–Ni alloys increases the interfacial energy. However, these alloying induced changes in $\sigma(9, n)$ are very small and thus the trends should be considered with precaution.

The present (9, 2) supercells are used in connection with equation (3) to find the SFE of Fe–Cr–Ni alloys. The results are listed in table 6. Our $\gamma$ values are in good agreement with the previous theoretical results [11, 12] and also with the limited number of experimental data [48–50]. Chromium is found to decrease the SFE and Ni slightly increases it, which is in line with the previous theoretical predictions [11–13].

Table 6, also shows the SFE obtained within the AIM and r-AIM (numbers in parentheses). It is interesting to notice that for the present mono-atomic systems (table 3) both the 1st and 3rd order AIM SFE values ($\gamma^{(1)}$ and $\gamma^{(3)}$) are larger than $\gamma$. For Al, Ni, Cu and Pt, the relaxed 1st order approximation ($\gamma^{0(1)}$) remains also above $\gamma$. The situation is very different for the steel alloys in table 6, for which we have $\gamma^{0(1)} < \gamma^{(1)} < \gamma^{(3)}$. This trend is reflected in the large positive pseudo-interfacial energies $\sigma^*$ obtained for all three alloys. Both Ni and Cr additions seem to decrease the pseudo-interfacial energy, although the variations are very small. Our predict pseudo-interfacial energies are slightly smaller than the values proposed by Olson and Cohen (10–15 mJ m$^{-2}$) [5].

For the present paramagnetic steel alloys, the 3rd order AIM performs reasonably well. Namely, the absolute difference between $\gamma^{(3)}$ and $\gamma$ is less than $\sim 6\%$, and most importantly, the alloying effects on the SFE predicted by the two methods are the same. In consequence, the interfacial energies $\sigma^{(3)}$ computed from the 3rd order AIM expression equation (9) are also close to $\sigma^*$. It is important to note that the trend of $\sigma^*$ is also well reproduced by the 3rd order AIM. However, when we omit the lattice distortion effect (2δ/A), the performance of the AIM ‘to predict’ the pseudo-interfacial energy is to a large extent ‘destroyed’. Unlike for the mono-atomic systems in table 3, in the case of steel alloys adopting the r-AIM scheme does not improve the agreement between the supercell and AIM results. The resulting composition dependence of the SFE is the same, but the corresponding SFE values are further underestimated compared to the supercell results.

3.3. Pseudo-interfacial energy versus coherent interfacial energy

Previously, we have briefly discussed the differences between the pseudo-interfacial energy $\sigma^*$ and the coherent interfacial energy ($\gamma$) as a function of supercell size $(m,n)$. Here we give a rigorous mathematical expression connecting these two interfacial energies and make an attempt to understand the origin of the differences between them. Using the definition of the coherent interfacial energy in equation (2), the SFE $\gamma(m)$ derived from the $(m,2)$ supercell (equation (3)) may be cast in the following form
\[ \gamma(m) = 2(F_{\text{hcp}}^{\text{SC}} - F_{\text{fcc}}^0)/A + 2\sigma(m, 2). \] (10)

Combining this expression with equation (1) (we recall that \( \gamma(m) \) converges to SFE with increasing \( m \)), we arrive at
\[ \sigma^* \cong \sigma(m, 2) + (F_{\text{hcp}}^{\text{SC}} - F_{\text{hcp}}^0)/A. \] (11)

According to that, the difference between the two interfacial energies is due to the different reference states for the hcp structure used in equations (1) and (2). Since the layer-relaxed hcp lattice always has higher energy than the equilibrium hcp lattice, the pseudo-interfacial energy should always be larger than the coherent interfacial energy computed for the \((m, 2)\) supercell. This effect is clearly seen from the calculated \( \sigma(m, 2) \) and \( \sigma^* \) values (tables 2, 3, 5 and 6). The difference between the two interfacial energies is given by the strain energy \((F_{\text{hcp}}^{\text{SC}} - F_{\text{hcp}}^0)/A\) which enters when matching coherently the hcp(0001) facet to the equilibrium fcc(11̄1) facet.

Comparing tables 2 and 3, we find that Cu, Ag and Ni have similar \( \sigma \) and \( \sigma(m, 2) \) values, the differences between them being less than \(-2.7 \text{ mJ m}^{-2}\). The small difference is due to the negligible \((F_{\text{hcp}}^{\text{SC}} - F_{\text{hcp}}^0)\) obtained for these metals (≤50 \( \mu \text{Ry per atom} \)). On the other hand, the rather large strain energy found for Pt makes the corresponding interfacial energies very different from each other (by about 18.2 \( \text{mJ m}^{-2} \)). It is clear that whenever the hcp lattice needs to be strongly deformed to match the fcc(1 1 1) facet, a sizable difference between the two interfacial energies is expected. In the case when the layer-relaxed hcp lattice is close to the equilibrium hcp lattice, the two interfacial energies should also be close to each other.

4. Conclusions
First-principles calculations have been performed to determine the intrinsic stacking fault energy and the fcc(1 1 1)/hcp(0001) interfacial energy for six elemental metals and three paramagnetic Fe–Cr–Ni alloys, which form the basic building block of austenitic stainless steels. For all systems, the predicted SFE results are in good agreement with the previous theoretical values and the available experimental data, confirming the accuracy of the present approach. The calculated interfacial energy is shown to depend strongly on the reference structures and chemistry.

We term the interfacial energy that enters the thermodynamical SFE calculations as the pseudo-interfacial energy \( \sigma^* \) with the equilibrium hcp and fcc structures as reference states. \( \sigma^* \) is determined according to the thermodynamical expression for SFE (equation (1)) using the calculated SFE. On the other hand, the coherent interfacial energy \( \sigma(\mathbf{9}, n) \) is defined as the excess energy at the coherent interface between semi-infinite fcc(11̄1) and hcp(0001) slabs. The results show that the coherent interfacial energy differs significantly from the pseudo-interfacial energy.

Contrasting the supercell results with those obtained using the axial interaction model allows us to study the performance of the AIM for interfacial energies. In terms of the AIM parameters, the pseudo-interfacial energy is simply given by the second order layer interaction plus a small correction lattice distortion term. Whenever the 3rd order AIM performs well for SFE, it also predicts the pseudo-interfacial energy \( \sigma^* \) with sufficient high accuracy. This is the case for Fe–Cr–Ni alloys, Cu, Ag and Au, and to lesser extend for AI and Ni. However, the 3rd order AIM fails for Pt, which might indicate the need to include higher order AIM interactions. No significant improvement is found when comparing the relaxed-AIM to the original AIM approximation.

For all elemental metals and Fe–Cr–Ni alloys considered here, \( \sigma(\mathbf{9}, n) \) is negative. Aluminum and platinum have the
largest $|\sigma(9,n)|$ values, whereas the noble metals and alloy steels have nearly vanishing coherent interfacial energies. The pseudo-interfacial energy shows large variations as we go from the simple metal Al to transition metals (Ni, Cu, Ag, Pt and Au) and transition metal alloys (Fe–Cr–Ni), which indicates that $\sigma$ strongly depends on chemistry. Our predicted pseudo-interfacial energies for the Fe–Cr–Ni alloys as slightly smaller than the commonly quoted values in the literature.

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