Martensitic transformations have been studied extensively due to their importance in applications for high-strength, shape-memory effects or superelastic properties. These are diffusionless first order solid-state transformations, which nucleate from a parent phase, commonly referred to as austenite. Martensite nucleates at a critical temperature $M_s$ (martensite-start) when the driving force for its nucleation is reached. Additional undercooling is required for the transformation to continue and reach completion at a temperature $M_f$ (martensite-finish). The reverse transition occurs upon heating the martensite to transform back to austenite; the temperatures at which the transformation begins and finish are austenite start ($A_s$) and finish ($A_f$), respectively. Although there are considerable studies in different alloying systems showing how martensite formation changes with composition [1–4], there is virtually no theoretical approximationable to predict the conditions for its occurrence without introducing fitting parameters or remaining valid in different phase transitions.

The objective of this work is to introduce a new approach to predict $M_t$ in systems undergoing the phase transitions: face-centred cubic (FCC) $\rightarrow$ body-centred cubic (BCC), FCC $\rightarrow$ hexagonal closed packed (HCP) and BCC$\rightarrow$HCP. The approach is based on determining the driving force for athermal martensite formation including energy terms of the transformation strains and lattice distortions by substitutional and interstitial atoms. The model has no adjustable parameters and it is able to predict $M_t$ and $A_t$ in Fe–Ti- and Co-based alloys, as well as the hysteresis cycle ($M_t$, $M_f$, $A_s$, $A_f$) in Co-based alloys.

Martensitic forms by the coordinated movement of atoms resulting in homogeneous shearing of the austenite and forming a new crystal structure without variations in chemical composition. The lattice correspondence between the austenite and martensite phases are nearly parallel to the most densely packed planes and their corresponding directions. This leads to the orientation relationships between the FCC, BCC and HCP phase transitions to be $\langle 111 \rangle_{\text{FCC}} \| \langle 110 \rangle_{\text{BCC}}$ and $\langle 110 \rangle_{\text{FCC}} \| \langle 111 \rangle_{\text{BCC}} \| \langle 112 \rangle_{\text{HCP}}$.

The phenomenological theory of martensite crystallography dictates that the transformation strain $\gamma_T$ consists of two components: a (Bain) strain distorting homogeneously the parent structure, and a lattice invariant strain $\tilde{\gamma}$ aiding in producing the correct shape of the martensitic structure. For the FCC$\rightarrow$BCC transition the transformation strain is computed by rotating the FCC unit cell, expanding two principal axes and compressing the remaining axis to correspond with the BCC unit cell [8]. Additional shearing of $\tilde{\gamma}=\sqrt{5}a_{\text{BCC}}-\sqrt{5}a_{\text{FCC}}$ along $\langle 110 \rangle_{\text{BCC}}$ is needed to achieve the correct shape. This is illustrated in Fig. 1(a), showing atoms in $\langle 111 \rangle_{\text{FCC}}\| \langle 110 \rangle_{\text{BCC}}$ (red) shuffle by $\frac{\sqrt{5}}{2}a_{\text{BCC}}$ (orange arrows) to reach the correct BCC shape (green). The principal strains to compute $\gamma_T$ are [8]:

$$\eta_1 = \frac{\gamma_T}{\sqrt{2/3}a_{\text{BCC}}} = \frac{\gamma_T}{\sqrt{2/3}a_{\text{FCC}}}$$

$$\eta_2 = \frac{\gamma_T}{\sqrt{1+\gamma_T}}$$

$$\eta_3 = \frac{\gamma_T}{\sqrt{1+\gamma_T}}$$

The transformation strain is: $\gamma_T = \sqrt{\eta_1^2 + \eta_2^2 + \eta_3^2}$. The principal strains of

$1$ These are idealised relations, however they have shown sufficient accuracy with experiments when determining various crystallographic parameters [5–7].
Fig. 1. Schematic representation of the atomic displacements in BCC ⇔ FCC, FCC ⇔ HCP and BCC ⇔ HCP transitions and their orientation relationships. (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.)

Table 1

| Transition   | \( \eta_1 \) | \( \eta_2 \) | \( \eta_3 \) | \( \gamma_T \) | \( |\Delta G_T| \) [J/mol] | Exp [J/mol] |
|--------------|--------------|--------------|--------------|--------------|-----------------|-------------|
| FCC ⇔ BCC    | \( \frac{1}{\sqrt{3}} \left[ 1 + \frac{1}{\sqrt{3}} \right] a \) | \( \frac{1}{\sqrt{3}} \left[ 1 + \frac{1}{\sqrt{3}} \right] a \) | \( \frac{1}{\sqrt{3}} a \) | 0.24 (Fe)      | 1255            | 1000–1250 [19–21] |
| BCC ⇔ FCC    | \( \frac{1}{\sqrt{2}} \left[ 1 + \frac{1}{\sqrt{2}} \right] a \) | \( \frac{1}{\sqrt{2}} \left[ 1 + \frac{1}{\sqrt{2}} \right] a \) | \( \frac{1}{\sqrt{2}} a \) | 0.17 (Fe)      | 500             |             |
| BCC ⇔ HCP    | \( \frac{1}{\sqrt{6}} \left[ 1 + \frac{1}{\sqrt{6}} \right] a \) | \( \frac{1}{\sqrt{6}} \left[ 1 + \frac{1}{\sqrt{6}} \right] a \) | \( \frac{1}{\sqrt{6}} a \) | 0.1014 (Ti) | 130             | 150 [3]     |
| FCC ⇔ HCP    | \( \frac{1}{\sqrt{2}} \left[ 1 + \frac{1}{\sqrt{2}} \right] a \) | \( \frac{1}{\sqrt{2}} \left[ 1 + \frac{1}{\sqrt{2}} \right] a \) | \( \frac{1}{\sqrt{2}} a \) | 0.026 (Co) | 18              | 35 [22]      |
| HCP ⇔ FCC    | \( \frac{1}{\sqrt{6}} \left[ 1 + \frac{1}{\sqrt{6}} \right] a \) | \( \frac{1}{\sqrt{6}} \left[ 1 + \frac{1}{\sqrt{6}} \right] a \) | \( \frac{1}{\sqrt{6}} a \) | 0.027 (Co) | 18.8            |             |

The BCC ⇔ FCC transition are computed by similar rotations and by shearing \( \frac{\sqrt{3}}{\sqrt{2}} [111]_{\text{BCC}} \) the lattice, with \( \delta = \frac{\sqrt{3}}{\sqrt{2}} \). Burger [9] followed a similar argument to compute the magnitude increasing to \( a_{\gamma} \left[ 1 + \frac{1}{\sqrt{3}} \right] = a_{\gamma} \left[ 1 - 2 \frac{\sqrt{3}}{\sqrt{2}} \right] \) and \( \eta_3 \) is [14]: \( \eta_3 = \frac{\sqrt{3}}{\sqrt{2}} a_{\gamma} \). The HCP ⇔ FCC transition has been argued to occur by the reverse process with analogous principal strains [13,14].
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