Understanding Solid–Solid (fcc $\rightarrow$ ω + bcc) Transition at Atomic Scale

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Abstract An atomic transition model of a face-centered cubic (fcc) crystal to a primitive hexagonal ω and body-centered cubic (bcc) structures has been crystallographically built. The fcc structure can transform into the ω structure through a local shuffling or displacement of atoms about 0.4014 Å in iron for $a_{\text{fcc iron}} = 3.59$ Å. The bcc structure can form either after the ω formation or concurrently by the similar mechanism, or the ω structure can be treated as an intermediate stage during the transition of fcc $\rightarrow$ bcc. Such a transition (fcc $\rightarrow$ ω + bcc transition) can be confirmed by Widmanstätten pattern formed in an iron meteorite, pearlitic structure and martensite composed of bcc-ferrite and ultra-fine ω particles in iron–carbon steels. The present fcc–bcc orientation relationship matches with Pitsch’s one.

KEY WORDS: Solid–solid transition; ω Transition; Martensitic steel; Modeling; Crystallography; Twin; Phase transformation

1 Introduction

In every case of steel, even up to the current society equipped with modern analysis techniques to an atomic-scale resolution, practice in metallurgy is still far ahead of steel science. Researchers in the steel field are still in a puzzle about the quenching hardening behavior in carbon steels (the steel containing certain amount of carbon or an Fe–C alloy becomes hard and brittle after a fast temperature reducing procedure from austenite temperature field to room temperature or lower) and ductile–brittle transition temperature (DBTT) (the metals or alloys become brittle after they pass a temperature interval) [1–5].

In 1885, a noted French metallurgist, Floris Osmond, postulated “ β -Fe or β -ferrite” in carbon steel as an allotrope of iron, which had the same crystal structure with α -ferrite (α -Fe with a body-centered cubic (bcc) structure) and been treated as a hardener phase [6, 7]. In the quenching of steel, “ β -Fe or β -ferrite” was “caught in transit” between high-temperature austenite (γ -Fe with a face-centered cubic (fcc) structure) and low temperature α -Fe and thereby played a vital part in the hardening of carbon steel [8]. In the early 1920s, such “ β -Fe” was completely denied by a proposed body-centered tetragonal (bct) martensite based on X-ray diffraction results on high carbon steels [9–13]. Since then, researchers tend to accept the bct martensite as a single crystalline phase and that the carbon atoms are trapped in the interstitial position of the bct structure during quenching process, which results in the quench hardening of carbon steel [3, 14, 15]. The bct or bcc martensite has been suggested to form directly from the high-temperature γ -Fe during cooling process. However, such direct phase transformation (normally called as “martensitic transformation” in current textbooks) of fcc $\Rightarrow$ bcc still causes a lot of controversy in steel science [1, 2].

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In carbon steel, in particular, high carbon steel, two-phase structure has been observed very recently in martensite by means of transmission electron microscopy (TEM) [16, 17]. These two crystalline phases are α -Fe (ferrite with bcc structure) and ω -Fe(C). The ω -Fe with a nanoscale particle-like morphology has a primitive hexagonal structure and can be stabilized by carbon atoms. Thus, the martensite is α -ferrite matrix phase embedded with a high density of ultra-fine ω -Fe(C) particles as a second crystalline phase.

The question about the formation mechanism of the martensite with two-phase structure ($\omega + \text{bcc}$) has naturally been risen. Thus, a preliminary idea to suggest the two-phase formation directly from the fcc austenite is necessary for understanding the phase transition in martensitic steels. The present modeling will suggest that it is possible for a fcc crystal to transform into $\omega + \text{bcc}$ structures crystallographically. The postulated transformation process can be applied for the explanation of a complex structure formed in iron and steel and also Widmanstätten pattern in iron meteorites.

2 The bcc $\rightleftharpoons \omega$ Transition

The bcc $\rightleftharpoons \omega$ transition, occurring via collapse of adjacent $(111)_{\text{bcc}}$ planes, has been well established in bcc metals and alloys [17–23] and yields the ω phase precipitates with the following orientation relationships to the parent bcc phase: $[1\bar{1}0]_{\text{bcc}} // [11\bar{2}0]_{\omega}$, $(112)_{\text{bcc}} // (1\bar{1}00)_{\omega}$, $(11\bar{1})_{\text{bcc}} // (0001)_{\omega}$; and $a_{\omega} = \sqrt{2} \times a_{\text{bcc}}$ and $c_{\omega} = \sqrt{3}/2 \times a_{\text{bcc}}$, as revealed in Fig. 1, which shows the projection of atoms in a bcc structure along $[1\bar{1}0]_{\text{bcc}}$ (Fig. 1a) and an atomic structure model of a primitive hexagonal ω crystal (Fig. 1b), and the ω unit cell in Fig. 1a can be viewed as the projection of Fig. 1b along the $[11\bar{2}0]_{\omega}$ zone axis. In Fig. 1a, the black

spots represent atoms in a $(1\bar{1}0)_{\text{bcc}}$ plane and the open circles represent atoms in the plane below or above; the bcc unit cell is outlined by green lines; the atoms outlined by red dashed lines are still in a bcc structure, but will transform into an ω unit cell with a primitive hexagonal structure, the red arrows indicate the direction of the atom movement or displacement (in a $\{112\}_{\text{bcc}}$ plane along one $\langle 111 \rangle_{\text{bcc}}$), and the shuffling distance is $(\sqrt{3}/12)a_{\text{bcc}}$; the atoms outlined by blue dashed lines are at an arrangement of an ω unit cell.

Since the ω formation is common in bcc metals and alloys by an atomic shuffling of about $(\sqrt{3}/12)a_{\text{bcc}}$, around 0.479 Å for a bcc Ti where $a = 3.32$ Å, it is reasonable to think that a similar shuffling may happen in fcc crystals. However, no any experimental observations have suggested that the ω phase existing in fcc metals and alloys to date. A recent finding that the martensitic structure in quenched Fe–C alloys and carbon steels is actually composed of bcc-ferrite matrix and a high density of ultra-fine ω particles has stimulated the author to think about the possibility of the ω formation in fcc metals and alloys [16, 17, 25].

3 Modeling

3.1 An ω Unit Cell in a fcc Crystal

Figure 2 shows the formation mechanism for a near-perfect ω unit cell in a perfect fcc crystal. Figure 2a is a three-dimensional hard-sphere structure model of a fcc crystal with an initial ω structure outlined in blue lines; all the atoms are in a perfect fcc arrangement at this stage. Figure 2b shows a projection of Fig. 2a along c axis, where a , b and c are the three axes of the fcc structure.

A near-perfect ω unit cell can be formed in the fcc lattice by an atomic shuffling or displacement, as shown in

Fig. 1 **a** Projection of atoms in a bcc structure along $[10]_{\text{bcc}}$; **b** an atomic structure model of a primitive hexagonal ω crystal

Fig. 2 **a** Atomic structure model of a fcc crystal; **b** projection of the fcc structure along $[001]_{\text{fcc}}$ zone axis; **c** projection of the near-perfect ω unit cell, which is formed in the fcc lattice by an atomic shuffling or displacement (black spots and the open circles represent the atoms in different $(001)_{\text{fcc}}$ planes (or c plane))

Fig. 2c, where the shuffling direction is indicated by arrows. It can be seen from Fig. 2c that the atoms outlined by dashed lines in Fig. 2b were shifted, and each arrow represents a movement or displacement of the corresponding atom along the arrow direction with a distance of $(\sqrt{5}/20)a_{\text{fcc}}$. One unit cell of an ω lattice after the shuffling of the corresponding atoms is shown by blue lines in Fig. 2c. It is also schematically shown in Fig. 2c that the corresponding shuffling distance is $(\sqrt{5}/20)a_{\text{fcc}}$, and it is about 0.4014 Å in fcc iron for $a_{\text{fcc}} = 3.59$ Å. All shuffling distances are equal. Such shuffling will result in an ω unit cell from the fcc iron matrix with a_{ω} is $\sim(\sqrt{5}/\sqrt{3})a_{\text{fcc}}$ (~ 4.64 Å), and c_{ω} is $\sim 3/(2\sqrt{5})a_{\text{fcc}}$ (~ 2.41 Å). Since no ω phase has been directly observed in fcc materials, the above lattice parameters are calculated based on the model shown in Fig. 2c. The depth distance of the ω unit cell shown in Fig. 2c is $1/2a_{\text{fcc}}$ (~ 1.795 Å), which is close to the depth distance, $1/2a_{\omega}$ (~ 2.025 Å), of the ideal ω structure shown in Fig. 1b.

Experimental results have revealed that the ω phase and bcc-iron in martensitic carbon steels have the same relationship as that in bcc-Ti alloys [16, 17, 25]. Thus, an experimentally observed ω phase in bcc-iron matrix has $a_{\omega} = \sqrt{2} \times a_{\text{bcc}} \approx 4.05$ Å and $c_{\omega} = \sqrt{3}/2 \times a_{\text{bcc}} \approx 2.48$ Å for $a_{\text{bcc}} = 2.86$ Å. The large value of a_{ω} is ~ 4.64 Å in modeling may be reduced during the relaxation processing from the near-perfect lattice to final experimental structure.

The ω structure in Fig. 2c can be easily extended in $(0001)_{\omega}$ plane, but the extension of ω structure along its c axis appears more difficult, as shown in Fig. 3. Figure 3

Fig. 3 Two perpendicular ω variants outlined by blue lines in one fcc crystal along $[001]_{\text{fcc}}$ zone axis, where the parallel two ω unit cells are belonged to one ω variant, and these ω variants cannot schematically be repeated along its c axis

also shows two perpendicular ω variants connecting to each other; such connection will ultimately leave an atom alone at the center of the above configuration. Simply speaking, the ω tends to form platelike structure with $(0001)_{\omega}$ plane as the plate plane. The growth in its thickness will be difficult and possibly follow a similar mechanism with the twinning growth by merging more twin plates together [26].

A fcc crystal grain could rapidly transform into an ω grain if the ω structure or unit cell could be easily extended along its c axis. The fact that the above transformation has never been experimentally observed in any metals and alloys suggests, therefore, that the ω phase can form plates of only one unit cell thickness easily; such an ω structure (or phase) only one unit cell in thickness is likely to be quite unstable thermodynamically and rapidly revert or convert to another phase. This serves as a probable reason for why the ω structure has not been observed in fcc crystals to date, as contrasted with the ω phase in bcc metals and alloys. Rather, ω instability may instead act to nucleate bcc structure formation in the corresponding fcc crystal, due to the reversible $\omega \leftrightarrow$ bcc transition.

3.2 Possible ω Variants in One fcc Crystal

Figure 4 shows four ω variants that may be formed in one fcc crystal, as viewed along the $[001]_{\text{fcc}}$ axis. Figure 4a shows two ω variants related by an angle of about 36.88° around the $[001]_{\text{fcc}}$ axis. Another two variants, shown in Fig. 4b, can be obtained by rotating the variants (in Fig. 4a) 90° around the $[001]_{\text{fcc}}$ axis. Thus, along one direction, the rotating angle among the four ω variants can be 36.88° , or 90° , or $90^\circ \pm 36.88^\circ$. One point that should be emphasized here is that one atom can shuffle in four directions equally in one atomic plane, as indicated by the arrows in Fig. 4a, b. One fcc crystal has three equal $\langle 100 \rangle$ directions; thus, the fcc crystal can have twelve ω variants formed at the same time. In Fig. 4a, b, the black atom at the intersection of the inner edge of the two ω variant unit cells has a tendency to shift via two

translation steps, which are nearly parallel to each other, if the two ω variants form at the same time. Such a chance occurs for every atom. If an atom can move two such translations in one direction, then the formation of a bcc unit cell in the fcc crystal will be possible.

3.3 One bcc Unit Cell in One fcc Crystal

Figure 5 shows a bcc unit cell formed in a fcc crystal with the help of the ω structure. If two parallel ω unit cells meet together, as shown in Fig. 5a, the four open circled atoms will automatically move to their current positions as outlined by dashed red lines, which indicate a bcc unit cell. In Fig. 5b, the presence of the other two ω unit cells will serve to assist the two black atoms' motion into their positions, as shown in Fig. 5c, which corresponds to their positions in the ω structure. Since the ω structure is quite unstable, the two black atoms may shuffle backward or forward to find their suitable positions; if they shuffle forward, then a bcc unit cell will form in one fcc crystal. Such a shuffling backward or forward mechanism has been postulated in the $\{112\}\langle 111 \rangle$ -type twinning in bcc metals and alloys [17, 26].

For simplicity, a pair of ω and bcc unit cells in one fcc crystal is shown in Fig. 6. Atoms indicated with the double arrows undergo a shuffling or displacement twice the distance implied by a single arrow. Such a double shuffling would be difficult without the ω structure. As with the ω structure, the bcc phase is restricted in its growth; the bcc can grow easily along the $\langle 111 \rangle_{\text{bcc}}$ directions in $\{112\}_{\text{bcc}}$ habit planes (a habit plane must be un-rotated and un-distorted), but is conversely unable to grow perpendicular to

Fig. 4 Four ω variants along one basal direction of a fcc crystal: **a** two ω variants with a rotating angle of about 36.88° ; **b** the other two ω variants

Fig. 5 A schematic formation mechanism of one bcc unit cell in a fcc crystal with the help of the ω structure: **a** two parallel ω unit cells meet together not in the same atomic plane; **b** another two parallel ω unit cells join in Fig. 5a; **c** one bcc unit cell formed

Fig. 6 A schematic illustration of a pair of one bcc unit cell and one ω unit cell in a fcc crystal along the $[001]_{\text{fcc}}$ direction

these planes. This is probably the physical reason of $\{112\}$ becoming the habit plane of bcc structure. The arrows related to the bcc structure formation should parallel to the $\{112\}_{\text{bcc}}$ plane and along $\langle 111 \rangle_{\text{bcc}}$ direction. The ω and bcc unit cells shown in Fig. 6 can be treated as nuclei for the homogeneous nucleation of the ω and bcc phases, while the growth of both ω and bcc in their thickness direction can be realized by overlapping the nuclei with each other when they meet together. Such a growth mechanism is similar to that of the $\{112\}\langle 111 \rangle$ -type twinning growth [26]. Furthermore, the dislocations, twins, cracks and other kinds of defects may be formed while the merging of those nuclei occurs too rapidly.

Finally, the fcc-bcc orientation relationship based on the present transformation mode matches well with Pitsch's

Fig. 7 Four pairs (A–D) of ω /bcc unit cells in one fcc crystal, where A-bcc and A- ω correspond to the bcc unit cell and the ω unit cell in the A-pair, respectively

one, which gives $(001)_{\text{fcc}} // (101)_{\text{bcc}}$, $[\bar{1}10]_{\text{fcc}} // [\bar{1}11]_{\text{bcc}}$, $[110]_{\text{fcc}} // [12\bar{1}]_{\text{bcc}}$ [27]. The Pitsch orientation relationship or Pitsch distortion has been suggested to be an earlier stage before Kurdjumov–Sachs (K–S) and Nishiyama–Wassermann (N–W) orientation relationships with respect to the fcc matrix [28]. In such a sense, the present discussed fcc $\rightarrow \omega$ transition is a very earlier stage than that Pitsch distortion suggested.

Figure 7 reveals four pairs of ω and bcc unit cell variants in one picture. Each bcc unit cell has two $\{112\}_{\text{bcc}}$ planes as indicated by dashed green lines. A 180° rotational

symmetry exists between variants A and D or variants B and C. There is one common or parallel $\{112\}$ plane between variants A and C, and similarly, there is one between variants B and D. A $\{112\}\langle 111 \rangle$ -type twin of bcc crystal may form between variants A-bcc and C-bcc since the bcc variant in C can overlap with the bcc variant in A after rotating 180° around the green dashed line ($\langle 111 \rangle$ direction in $\{112\}$ plane) in C. The same thing can happen between B and D. This may be the origin of transformation $\{112\}\langle 111 \rangle$ -type twins formed in twinned martensitic steel. The above formation mechanism of bcc and ω in one fcc crystal is simply called as “fcc $\rightarrow \omega + \text{bcc}$ transition” in the present postulated modeling.

4 A near-Perfect bcc Structure in a fcc Crystal

Based on the above analysis, a near-perfect bcc unit cell in one fcc structure can be simply illustrated in Fig. 8a. The black and blue spots together with the B, O and B' red spots are the atoms in a fcc structure. Those red atoms are forming a near-perfect bcc structure. The shuffling/displacement direction and distance of the atoms are indicated in green arrows and double arrows mean that the atom shuffled two times of one arrow distance, which is equal to $(\sqrt{5}/20)a_{\text{fcc}}$. The near-perfect bcc structure is independently shown in Fig. 8b. This near-perfect bcc structure will have lattice parameters: $a = b \approx 2.732 \text{ \AA}$ and $c \approx 2.969 \text{ \AA}$, which will give a lattice strain of around 3.8% with reference to a perfect bcc with $a \approx 2.86 \text{ \AA}$. Relaxation among the atoms in Fig. 8b may result in the formation of a perfect bcc lattice. Figure 8b is only one near-perfect bcc variant, and another variant can be obtained by shuffling those atoms in the opposite direction; if A, O and A' atoms remain un-shuffling, the similar shuffling behaviors of A and A' atoms happen on B and B'

atoms, then other two variants can be obtained. Along one axis of the fcc structure, four bcc variants can be formed. Thus, twelve bcc variants will be formed in one fcc crystal due to that a cubic crystal has three perpendicular axes.

5 The Applications of the “fcc $\rightarrow \omega + \text{bcc}$ Transition”

5.1 The Formation of Pearlitic Lamellar Structure

The model for the ω and bcc structure formed in a fcc crystal shown in Figs. 6 and 7 matches well with an experimental observation of the pearlite lamellar structure in carbon steels [29–31], where the bcc ferrite has its habit plane of $\{112\}_{\text{bcc}}$ in the pearlite lamellar structure. As it can be seen in Figs. 6 and 7, the bcc structure can form a platelike structure in planes parallel to the $\{112\}_{\text{bcc}}$ planes. Here, if the ω structure is enriched with enough carbon atoms, carbon is a ω structure stabilizing element in carbon steel [16], then the ω phase will be remained not to help or serve for the bcc structure formation (here, once the ω structure serves for the bcc structure formation, the ω structure is usually quite unstable and will not be remained; if the ω structure can be remained, then those ω cannot serve as a nucleation site for the bcc structure formation). The ω phase with enough carbon atoms will easily transform into cementite ($\theta\text{-Fe}_3\text{C}$) particles energetically [16]. Thus, a lamellar pearlitic morphology, with one layer of ferrite and one layer of cementite (the layer of cementite is usually a segregation of fine $\theta\text{-Fe}_3\text{C}$ particles), can be formed in carbon steels if the cooling rate is slow enough. If the cooling rate is fast enough, however, then a so-called martensite structure will be formed; in the martensite, a high density of ultrafine particle-like ω embedded in the ferrite matrix has been recently explored [16, 17, 25].

Fig. 8 **a** A near-perfect bcc structure (red spots) in an ideal fcc crystal (black and blue spots and the red spots at B, O and B' positions), where each green arrow represents a movement or displacement of the corresponding atom along the arrow direction which is paralleled to the B–O–B' line with a distance of $(/20)a_{\text{fcc}}$; **b** the near-perfect bcc lattice structure withdraws from **a**; the distance among the atoms and the angle among various planes have been calculated based on $a_{\text{fcc}} = 3.59 \text{ \AA}$

Fig. 9 Transmission electron microscope image taken along the $[110]$ zone axis of ferrite from a furnace cooled Fe-0.7 wt% C plate sample with a thickness of about 2 mm after treated at 1100 °C for 1 h; the inset is the corresponding selected area electron diffraction pattern

The pearlite in carbon steels is not only formed in a lamellar structure; instead, some local regions with a short bar or plate of cementite can often be observed, as given in Fig. 9. Figure 9 is a bright field transmission electron micrograph (TEM) revealing that rodlike cementite particles can occur in ferrite. The image was taken with the electron beam parallel to the $[110]$ zone axis of bcc ferrite, as revealed by the inset electron diffraction pattern in Fig. 9. This is the same alignment used to draw the bcc structures shown in Figs. 6 and 7. Most of the cementite rods in the picture are aligned along the five red lines, which differ by angles of 90° , 53° and/or 37° , and these angles match perfectly with the angles among those ω variants in Fig. 4. Taking into account the ω and bcc variants (one ω variant can correspond to one bcc variant) as shown in Fig. 4, such disconnected cementite with a rotation angle can be treated as a competitive result among those variants during the nucleation and growth period. Of course, the lamellar structure of pearlite is also a competitive result of the variants. When Fe–C alloys experience a slow cooling rate, then one of the variants (ω and/or bcc) tend to establish growth first and ultimately dominate the resulting material. However, increasing the cooling rate results in a loss of such priority and the occurrence of the competitive growth among all the variants; this is a possible formation mechanism of the martensitic structure, which reveals a high density of ultra-fine (several nanometers) particle-like ω embedded in a bcc-Fe matrix, in carbon steels after fast cooling.

One interesting result that has been noticed is that there are five variants observed in Fig. 9. The extra variant may be the projection of the variant belongs to other directions since the observed TEM specimen has a certain thickness

(several tens of nanometer to several hundreds of nanometer). Dislocation-like defects connecting those cementite rods in the ferrite matrix can be clearly observed in the TEM image. These defects are most likely the merging product of the bcc domains with the same variant, which means that two or more bcc domains with an exact same orientation relationship with respect to the fcc matrix meet together, and possible impurity elements may remain at the meeting boundary (dislocation-like defect). As shown in Fig. 7, grain boundaries may be formed when different bcc variants meet together during slow cooling. If the variants A and B or C and D meet together very fast, a crack may form due to the two bcc variants are perpendicular to each other and the atoms in the front of the meeting variants do not have enough time to adjust their positions to fit each other.

5.2 Widmanstätten Structure in Iron Meteorites

The present modeling of fcc transforming into ω and bcc also matches well with Widmanstätten structure formed in an iron meteorite [32]. The optical micrograph of a slice of a specimen of the Gibeon meteorite cut (nearly) parallel to the (001) plane in Ref. [32] has revealed two variants of bcc plates perpendicular to each other; the bcc plates are called as Widmanstätten structure. The traces of Widmanstätten plates are parallel to two $\langle 110 \rangle_{\text{fcc}}$ directions. Those two perpendicular plates correspond to the bcc variants (A-bcc and B-bcc) or (C-bcc and D-bcc) as shown in Fig. 7. In Fig. 7, the habit plane of A-bcc or C-bcc variant is perpendicular to that of B-bcc or D-bcc variant, respectively. These bcc habit planes ($\{112\}_{\text{bcc}}$) are parallel with the $\{110\}$ planes of the fcc structure as shown in Fig. 7. Such a proposed result matches with the experimental observation from the iron meteorite. Iron meteorite contains less carbon atoms [33, 34]; thus, the ω phase cannot be retained unlike in quenched Fe–C system, in which both ω and bcc phases can be observed.

5.3 The Formation of Martensitic Structure in Carbon Steels

In fast-cooled Fe–C alloys, martensitic structure consisting of bcc-ferrite matrix phase and a high density of ultra-fine ω -Fe(C) particles has been observed [16, 17, 25]. It is also noticed that there is only one ω variant existing in the bcc-ferrite matrix with or without the $\{112\}\langle 111 \rangle$ -type twin by TEM observations (bcc and its $\{112\}\langle 111 \rangle$ -type twin are two variants of bcc structure). Unlike the ω phase precipitated from bcc matrix, where two variants of that kind of ω phase could be observed along one zone axis of the matrix phase in bcc metals and alloys including high alloying bcc steels [18–24, 35–39]. The TEM observations

on the martensitic substructure of quenched Fe–C alloys have revealed that only one ω variant can be seen along one zone axis of the ferrite matrix phase [16, 17, 25].

As revealed in Fig. 7, four ω /bcc variants should exist at the same local region. In fact, experimental results have revealed the existence of the A-bcc and B- ω , or A-bcc and C-bcc (C-bcc has a twinning relationship with A-bcc) and B- ω , or A-bcc and C-bcc and D- ω , or C-bcc and D- ω . Simply speaking, the ω pairs shown in Fig. 4a and b (or A- ω and C- ω ; B- ω and D- ω in Fig. 7) have never been observed at the same local region in fast-cooled Fe–C system. A possible reason is the difference of the displacement direction of the local atoms. As revealed in Fig. 7, in A- ω and B- ω variants, the local atoms are in the same behavior of a collective movement as indicated by the dashed green circle and arrows; however, an opposite collective behavior of the local atoms is noticed for C- ω and D- ω variants as indicated by the dashed red circle and arrows. Thus, it is reasonable for A- ω and B- ω or C- ω and D- ω instead of A- ω and C- ω or B- ω and D- ω appear in a local region. Such a local collective movement is possible to be a diffusion way for the atom diffusion in a solid crystal without any vacancy.

Since carbon atoms can stabilize the ω structure, in such a case, if A- ω is stabilized, then no A-bcc can be formed; if B- ω or D- ω is not stabilized, they will serve for the bcc or bcc-twin structure formation. Thus, only one ω variant can be detected in local regions.

A similar simple explanation can be proposed based on Fig. 5. In Fig. 5a, only one ω variant coexists with a bcc unit. In Fig. 5b and c, there is another ω variant, which is perpendicular to the one shown in Fig. 5a. However, if this second ω variant is stable, then the bcc unit cannot be formed. Thus, only the configuration shown in Fig. 5a can exist in materials, i.e., only one ω variant can coexist with a bcc lattice structure and their orientation relationship also matches with that observed in experiments.

6 Summaries

A primitive hexagonal ω structure can form in fcc crystals. The ω instability can help or serve to bcc structure formation in fcc crystals. A fcc crystal can transform into $\omega + \text{bcc}$ structure (fcc $\rightarrow \omega + \text{bcc}$ transition) crystallographically. The fcc $\rightarrow \omega + \text{bcc}$ transition can be treated as an earlier stage than that Pitsch distortion suggested.

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References

- [1] O.D. Sherby, J. Wadsworth, D.R. Lesuer, C.K. Syn, Mater. Trans. **49**, 2016 (2008)
- [2] O.D. Sherby, J. Wadsworth, D.R. Lesuer, C.K. Syn, Mater. Sci. Technol. **28**, 471 (2012)
- [3] M. Cohen, Trans. TMS AIME **224**, 638 (1962)
- [4] G. Krauss, Mater. Sci. Eng. A **273–275**, 40 (1999)
- [5] J.W. Christian (ed.), *Theory of Transformations in Metals and Alloys* (Pergamon Press, Oxford, 1965)
- [6] F. Osmond, J. Werth, Annales des Mines **8**, 5 (1885)
- [7] M. Cohen, J.M. Harris, in *The Sorby Centennial Symposium on the History of Metallurgy*, ed. by C.S. Smith (Gordon and Breach Science Publishers, New York, 1965), pp. 209–233
- [8] H.M. Howe (ed.), *Metallography of Steel and Cast Iron* (McGraw-Hill, New York, 1916)
- [9] A. Westgren, G. Phragmen, J. Iron Steel Inst. **103**, 303 (1921)
- [10] A. Westgren, G. Phragmen, J. Iron Steel Inst. **105**, 241 (1922)
- [11] W.L. Fink, E.D. Campbell, Trans. Am. Soc. Steel Treat. **105**, 241 (1926)
- [12] P.P. Ewald (ed.), *Fifty Years of X-ray Diffraction* (N.V.A. Oosthoek's Uitgeversmaatschappij, Utrecht, 1962)
- [13] K.H. Jack, J. Iron Steel Inst. **169**, 26 (1951)
- [14] E.C. Bain, in *The Sorby Centennial Symposium on the History of Metallurgy*, ed. by C.S. Smith (Gordon and Breach Science Publishers, New York, 1965), pp. 121–138
- [15] J.R. Davis (ed.), *Metals Handbook* (ASM, Materials Park, 1998)
- [16] D.H. Ping, W.T. Geng, Mater. Chem. Phys. **139**, 830 (2013)
- [17] D.H. Ping, Acta Metall. Sin. (Engl. Lett.) **27**, 1 (2014)
- [18] P.D. Frost, W.M. Parris, L.L. Hirsch, J.R. Doig, C.M. Schwartz, Trans. Am. Soc. Met. **46**, 1056 (1954)
- [19] B.A. Hatt, J.A. Roberts, G.I. Williams, Nature **180**, 1406 (1957)
- [20] J.M. Silcock, Acta Metall. **6**, 481 (1958)
- [21] B.S. Hickman, J. Mater. Sci. **4**, 554 (1969)
- [22] S.L. Sass, Acta Metall. **17**, 813 (1969)
- [23] S.K. Sikka, Y.K. Vohra, R. Chidambaram, Prog. Mater. Sci. **27**, 245 (1982)
- [24] L.M. Hsiung, D.H. Lassila, Acta Mater. **48**, 4851 (2000)
- [25] D.H. Ping, J. Yin, W.Q. Liu, Y.J. Su, L.J. Rong, X.Q. Zhao, Acta Metall. Sin. **49**, 769 (2013). In Chinese
- [26] S.Q. Wu, D.H. Ping, Y. Yamabe-Mitarai, W.L. Xiao, Y. Yang, Q.M. Hu, G.P. Li, R. Yang, Acta Mater. **62**, 122 (2014)
- [27] W. Pitsch, Philos. Mag. **4**, 577 (1959)
- [28] C. Cayron, Acta Cryst. A **69**, 498 (2013)
- [29] W. Pitsch, Acta Metall. **10**, 79 (1962)
- [30] D.S. Zhou, G.J. Shiflet, Metall. Trans. A **23**, 1259 (1992)
- [31] N. Zhong, X. Wang, Z. Guo, Y. Rong, J. Mater. Sci. Technol. **27**, 475 (2011)
- [32] H.J. Bunge, W. Weiss, H. Klein, L. Wcislak, U. Garbe, J.R. Schneider, J. Appl. Cryst. **36**, 137 (2003)
- [33] A.J. Campbell, M. Humayun, Geochim. Cosmochim. Acta **69**, 4733 (2005)
- [34] J.T. Wasson, Geochim. Cosmochim. Acta **75**, 1757 (2011)
- [35] C.Y. Cui, D.H. Ping, J. Alloys Compd. **471**, 248 (2009)
- [36] G. Shao, P. Tsakiroopoulos, Acta Mater. **48**, 3671 (2000)
- [37] A.F. Yedneral, M.D. Perkas, Phys. Met. Metall. **33**, 89 (1972)
- [38] R. Ayer, L.P. Bendel, V.F. Zackay, Metall. Trans. A **23**, 2447 (1992)
- [39] C. Djega-Mariadassou, L. Bessaia, C. Servant, Phys. Rev. B **51**, 8830 (1995)