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Viewpoint Paper

Stacking fault tetrahedra in metals

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Abstract—Mechanisms for the formation of stacking fault tetrahedra in metals are critically reviewed in the light of recent observations, where it is claimed, incorrectly, that for the first time stacking fault tetrahedra have been observed, which are formed by a dislocation mechanism, without the involvement of vacancies. In this note the experimental conditions where stacking fault tetrahedra have been observed are defined, together with the mechanisms that have been put forward to explain the observations. Three fundamentally different mechanisms are identified.

Keywords: Stacking fault tetrahedra; Vacancies; Dislocations

Stacking fault tetrahedra (SFT) were first observed in samples of quenched gold, by Silcox and Hirsch in 1959 [1]. They suggested that the tetrahedra were formed by the clustering of the quenched-in vacancies to produce a faulted loop of $\mathbf{b} = 1/3\langle 1\,1\,1\rangle$, which dissociated along the three $\langle 1\,1\,0\rangle$ directions in the $\{1\,1\,1\}$ plane of the loop. The final defect was thus a closed defect, with stair rod dislocations along the edges of the tetrahedron and stacking faults on all four $\{1\,1\,1\}$ planes. There has been considerable debate as to whether such tetrahedra are in fact formed from a 3-D vacancy cluster of four vacancies, followed by growth involving jog lines (which are formed on the faces of the tetrahedron, by the absorption of vacancies), or if the initial vacancy cluster is indeed a dislocation loop of $\mathbf{b} = 1/3\langle 1\,1\,1\rangle$. In the absence of direct observation of nucleation and growth, the mechanism by which the tetrahedra form in quenched gold is not certain, but what is not disputed is that the tetrahedra are formed by the clustering of vacancies. SFT have also been observed in situ in electron-irradiated metals (e.g. [2]) using high-voltage electron microscopy. It is also accepted that they are formed by vacancy clustering, the more mobile interstitials, which are formed during electron irradiation, being eliminated at the free surface of the thin samples.

SFT were subsequently observed in many pure metals and alloys that had been deformed at room and higher temperatures [3]. These tetrahedra were up to 200 nm in edge length and this, together with the fact that the dislocations generated during deformation would act as sinks for any vacancies formed during deformation, was used as an argument that it was unlikely that the tetrahedra were formed by clustering of vacancies. In addition, it was found that the lower the stacking fault energy the larger the largest tetrahedron in the various alloys, and triangular loops of $\mathbf{b} = 1/3\langle 1\,1\,1\rangle$ were also observed in some of these deformed samples, the smallest of which was larger than the largest tetrahedron in that alloy. These observations suggested that the Silcox–Hirsch mechanism was involved and that loops of $\mathbf{b} = 1/3\langle 1\,1\,1\rangle$ were formed which, below a certain edge length (governed by the stacking fault energy), formed SFT. On the assumption that the SFT were formed via the Silcox–Hirsch mechanism, these observations were used to derive stacking fault energies, which were in reasonable agreement with other measurements. The mechanism put forward involved long jogs that would have to be formed by intersection, and that this was followed by slip of a partial dislocation to form a loop of $\mathbf{b} = 1/3\langle 1\,1\,1\rangle$, as illustrated in Figure 1.

Later, it was shown [4] that the same mechanism could operate if two dislocations interacted to produce a length of dislocation of $\mathbf{b} = \frac{1}{2}\langle 1\,1\,0\rangle$ along the $\langle 1\,1\,0\rangle$ at right angles to its Burgers vector, since cross slip and glide of the interacting dislocations could lead, via appropriate dissociation, to the formation of a loop of $\mathbf{b} = 1/3\langle 1\,1\,1\rangle$. This mechanism is perhaps more likely than the mechanism involving intersection, because jogs up to 200 nm would be difficult to form since they require continued intersection by a secondary slip dislocation. Importantly, it was explicitly concluded that vacancies were not involved, and for many years this has been the accepted view for tetrahedra formed in deformed metals. This conclusion is contrary

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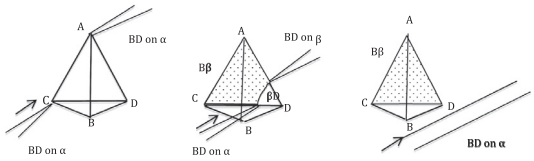

Fig. 1. Diagram, taken from Loretto et al. [3], showing the successive stages in the formation of a triangular Frank dislocation loop of Burgers vector **Bβ**. The jog along AC is perpendicular to the Burgers vector **BD**, which can dissociate to form **Bβ** and **βD**. The shaded regions are faulted by slip of the partial dislocation **βD** on beta. The arrow denotes the positive direction along the dislocation **BD**.

to many statements made in the paper by Wang et al. [5]. For example, among other assertions they state:

(i) "All of the stacking fault tetrahedra experimentally observed to date are believed to originate from vacancies". (ii) "The presence of vacancies that is critical for the initiation of SFT in the bulk". (iii) "On the other hand our discovery also provides an example of the deformation-induced and dislocation-originated formation mechanism of SFT in contrast to the conventional wisdom of vacancy-originated SFT…".

The present note has been triggered in part by the paper by Wang et al. but, more importantly, in view of work published long after the classic paper by Silcox and Hirsch, it seems apposite to assess critically the many observations of SFT which have been reported and to consider the various mechanisms that have been suggested for their formation. It is concluded in this viewpoint that three totally distinct mechanisms exist for the production of SFT.

The mechanism put forward by Wang et al. (which, it is argued below, cannot produce SFT) is based on direct observations made using high-resolution electron microscopy (HREM) of gold nanocrystals during tensile deformation. Figure 2, which is Figure 2(g) from Wang et al.'s paper [5], is reproduced below, where the stacking faults on β, γ and δ were observed to be formed by partial dislocations gliding in from the surface of the nanocrystal.

The faults on these inclined planes would be eliminated if the partial dislocations of $\mathbf{b} = \boldsymbol{\beta}\mathbf{C}$, **δB** and **γD**, also seen by Wang et al. to be generated from the free surface, were to glide towards the apex of the partial tetrahedron, as noted by Wang et al. They suggest, however, that one of these partials cross slips onto alpha and via various subsequent interactions, eventually produces an SFT. In the following discussion it is shown that the sequence of events suggested by Wang et al. cannot produce an SFT. Thus if, following Wang et al., it is assumed that any one of these dislocations, e.g. the dislocation with $\mathbf{b} = \boldsymbol{\beta}\mathbf{C}$, cross slips onto alpha, it would produce a stair rod dislocation of $\mathbf{b} = \boldsymbol{\beta}\boldsymbol{\alpha}$ along DC, which would involve an increase in energy, of about 30% if it is assumed that the energy of a dislocation is proportional to the magnitude of the square of the Burgers vector, because of the necessity of producing a stair rod dislocation. The reaction along DC is thus

$$\boldsymbol{\beta}\mathbf{C} \rightarrow \boldsymbol{\beta}\boldsymbol{\alpha} + \boldsymbol{\alpha}\mathbf{C}. \quad (1)$$

Wang et al. suggest, however, in their Supplementary information that if such cross slip occurs, this will lead to the generation of three partial dislocations (but no stair rod), as in Eq. (2),

$$\mathbf{C}\boldsymbol{\beta} \rightarrow \mathbf{B}\boldsymbol{\alpha} + \mathbf{C}\boldsymbol{\alpha} + \mathbf{D}\boldsymbol{\alpha} \quad (2)$$

This reaction is energetically far more unfavourable than that shown in Eq. (1), with one partial dislocation producing three new partial dislocations (four if a stair rod is included), so that the energy is increased by a factor of over three, though no reason for such an unlikely reaction is suggested. Wang et al. suggest that these three partial dislocations (which it must be presumed are closed loops) interact with the partial dislocations on the inclined {1 1 1} planes and thus produce a closed SFT, even though one of them, the dislocation of $\mathbf{b} = \mathbf{C}\boldsymbol{\beta}$, has cross slipped onto alpha, as shown in Eq. (2). It is not difficult to show that glide of these three partial dislocations on alpha cannot lead to the formation of an SFT. Hence this mechanism is considered no further.

If, however, reaction (1) takes place, the partial dislocation of $\mathbf{b} = \boldsymbol{\alpha}\mathbf{C}$ is glissile on alpha and could in principle react with the partial dislocations along DB and CB, as shown in Figure 3(a) and (b) and described in Eqs. (3) and (4). Note that in Figure 3(b) the positive directions of the dislocations are in opposite senses when they are

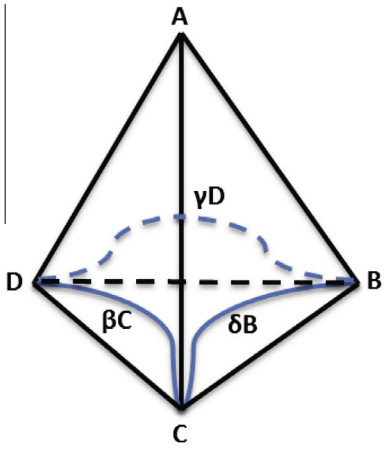

Fig. 2. Diagram, taken from Wang et al. [5], showing dislocations of $\mathbf{b} = \boldsymbol{\beta}\mathbf{C}$, **δB** and **γD** on the faulted {1 1 1} planes. The notation defining the Burgers vectors of dislocations is that of Thompson [6].

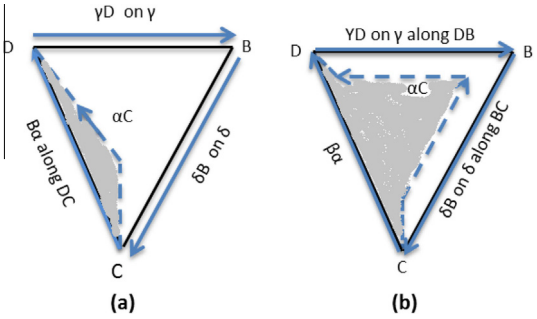

Fig. 3. Plan view of alpha viewed from A. The arrows indicate the positive sense of the dislocations. The shaded regions indicate that this area is faulted by glide of **αC** on alpha. (a) The situation after the dislocation: **βC** on beta has cross slipped onto alpha, producing the dislocation **αC** (shown as dashed) on alpha and the stair rod dislocation of $\mathbf{b} = \boldsymbol{\beta}\boldsymbol{\alpha}$. (b) The dislocation **αC** (shown as dashed) has slipped on alpha to be parallel to DB and BC, where it could react with the partial dislocations **γD** and **δB**.