Giant Atomic Clusters Induced Mechanism in \{10\bar{1}4\} Twinning of Hexagonal Close-Packed Crystals

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Following the discoveries of the giant atomic clusters (GACs) induced mechanism in a series of twinning modes in hexagonal close-packed (HCP) crystals, the law of atomic motion in hexagonal close-packed crystals, twinning, atomic clusters, mechanism, modeling

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1. Introduction

As well known, twinning is a primary plastic deformation mode that remarkably controls the mechanical behaviors of many materials and performs a vital role especially in HCP materials due to their limited independent slip systems.\(^1\)-\(^3\) As a basic issue for the twinning mechanism in the HCP crystals, the law of the atomic motion during twinning has long been a focus of attention.\(^4\)-\(^6\) Though quite a few research works were launched to make breakthrough in the past decades,\(^7\)-\(^9\) the progress is at a slow pace. In the early times, twinning shear was normally employed to judge the difficulty degree of a twinning mode to occur. But the hypothesis is challenged by some special cases, for example, as for magnesium, \{1013\} twinning occurs more infrequently than the \{10\bar{1}1\} twinning in spite of their equivalent twinning shears. Owing to the limitation of the “shearing” mechanism in the explanation of these cases, the “shuffle” mechanism emerged as the times require.\(^10\),\(^11\) But the interpretation of the shuffling mechanism itself becomes another intractable issue for its complexity and incapability in clarifying the process of atomic motion during twinning. With the rapid development of electron microscopy technique, plenty of cases based on the “dislocation” concept had been performed, by which the twinning mechanisms were attributed to the glide of defects (TD) called “twinning dislocations”\(^12\)-\(^14\) or “twinning disconnections”\(^15\),\(^16\) on their twin planes. Although these works had greatly broadened the knowledge to the twinning mechanism, they had not yet revealed the details of atomic motion in the twinning process.

On account of the above dilemma, the starting point originated in our early work,\(^17\) compared with the traditional treatment, was transformed by combining specified shearing and shuffling atoms as a whole to consider, but this slight change of analysis angle gave rise to an unexpected aspect that subverts the traditional ideas. We found in theory a stable atomic combination composed of massive shearing atoms and shuffling atoms serve as “medium” to induce twinning And by using this model, \{10\bar{1}2\}, \{10\bar{1}1\} and \{10\bar{1}3\} twinning were satisfactorily explained.\(^18\)-\(^20\) In this paper, \{10\bar{1}4\} twinning (K\(_1\) = \{10\bar{1}4\}, K\(_2\) = \{10\bar{1}0\}, \eta_1 = \{021\} and \eta_2 = \{0001\}), a mode with rather large value of shear (e.g., 0.937 in Mg),\(^1\),\(^21\) is explained by the GACs model. The atomic motion in this twinning mode is theoretically ascribed to the specified rotary motion of the GACs, which not only greatly simplified the explanation for this twinning mechanism in atomic scale, but also conversely consolidates the universality of the GACs induced mechanism in the HCP crystals.

2. Calculation

The atomic motion during the \{10\bar{1}4\} twinning in magnesium, a most typical HCP crystal lattice, is illustrated in Fig. 1. The shearing planes are numbered to distinguish the position of the shearing atoms: the one at the twin boundary are numbered as “0” and from which to the distant “1, 2, …, n”, thus the “kth” one is expressed as P\(_k\) (others similar). For the sake of the simplification of calculation, a rectangular coordinate system is constructed in the HCP crystal lattice (lower right corner of Fig. 1), and only a part of representative atoms surrounded by parallelogram “ABCD” and “EFGH” are selected to discuss (Fig. 2). The positions of the atoms after twinning are determined by the symmetric relation between the twin and the matrix.

The axial ratio of magnesium satisfies: \(\gamma = c/a = 1.623\) (here \(a\) and \(c\) are the basic crystal cell parameters). Thus the displacement vectors of these selected atoms can be calculated as follows:

\[
\begin{align*}
\mathbf{v}_A &= \mathbf{v}_{P1} = \Delta x_{A1} + \Delta y_{A1} + \Delta z_{A1} \\
&\approx 0ai - 0.624aj - 0.292ak \\
\mathbf{v}_B &= \Delta x_{B1} + \Delta y_{B1} + \Delta z_{B1} \\
&\approx 0ai - 0.889aj - 0.146ak \quad (1) \\
\mathbf{v}_C &= \Delta x_{C1} + \Delta y_{C1} + \Delta z_{C1} \\
&\approx 0ai - 0.825aj + 0.151ak \quad (2)
\end{align*}
\]

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the shearing atoms in the general formula for calculating the displacement vectors of along the $x$-

\[ \vec{v}_A = \Delta x A i + \Delta y A j + \Delta z A k \]

\[ \approx 0 a i - 0.566 a j + 0.005 a k \] (4)

\[ \vec{v}_E = \Delta x E i + \Delta y E j + \Delta z E k \]

\[ \approx 0 a i - 1.247 a j - 0.584 a k \] (5)

\[ \vec{v}_F = \Delta x F i + \Delta y F j + \Delta z F k \]

\[ \approx 0 a i - 1.513 a j - 0.432 a k \] (6)

\[ \vec{v}_G = \Delta x G i + \Delta y G j + \Delta z G \]

\[ \approx 0 a i - 1.455 a j - 0.141 a k \] (7)

\[ \vec{v}_H = \Delta x H i + \Delta y H j + \Delta z H k \]

\[ \approx 0 a i - 1.189 a j - 0.287 a k \] (8)

\[ |\vec{v}_{A1}| \approx 0.689 a \] (9)

where $\vec{v}_A$ is the displacement vector of atom $A$; $\vec{v}_{P1}$ is the displacement vector of the atoms on the twinning plane $P_1$; and $\Delta x_A, \Delta y_A$ and $\Delta z_A$ are the vector components of atom $A$ along the $x, y$ and $z$ axes respectively (others similar). Note that $\vec{v}_A$ is the minimum shearing vector of all, if the interplanar spacing of the [10\overline{4}] planes is defined as $d_A$, then twinning shear $s_A$ is obtained:

\[ s_A = \frac{|\vec{v}_{A1}|}{d_A} \approx 0.689 a \frac{0.735 a}{0.937} \approx 0.735 a \approx 0.937 \] (10)

Because of the periodicity of the twinning cells, the general formula for calculating the displacement vectors of the shearing atoms in the [10\overline{4}] twinning satisfies:

\[ \vec{v}_{P_k} = k \vec{v}_{P1} = k \vec{v}_A \] (11)

where $k = 0, 1, 2, \ldots n$ ($n$ is the sum of the twinning planes).

3. Discussion

The identification of atomic clusters is similar to the above-mentioned twinning modes (17-20) and no longer stated at length here. As shown in Fig. 2, four column of close packed atoms represented by atoms $A, B, C$ and $D$ compose.

one atomic cluster, so do the four columns represented by $E, F, G$ and $H$. The space structure of them is illustrated in Fig. 3, as can be seen which is composed of massive (e.g., hundreds of thousands in a coarse grain with size of 10 $\mu$m) octahedrons with their edges connected. For this reason, here this special structure is named “giant atomic clusters (GACs)”. The rotational angle of the GAC “ABCD” is obtained:

\[ \alpha_i \approx 20.2^\circ \] (12)

And the misorientation between the twin and the matrix in [10\overline{4}] twinning is:

\[ \beta_i \approx 50.2^\circ \] (13)

Since the atomic motion in [10\overline{4}] twinning can be ascribed to the rotational motion of the GACs, the difficulty degree of twinning can be understood is decided by the value of relative displacement magnitudes (RDMs) among the adjacent GACs. The relative displacement vectors between the atoms of unit “ABCD” and its adjacent atomic groups can be calculated as follows:

\[ \vec{v}_G - \vec{v}_A = (\Delta x_G - \Delta x_A) \hat{i} + (\Delta y_G - \Delta y_A) \hat{j} + (\Delta z_G - \Delta z_A) \hat{k} \]

\[ \approx 0 \hat{i} - 0.831 a + 0.151 a k \] (14)

thus the value of RDM in [10\overline{4}] twinning is obtained:
Since the value of the RDM reflects the degree of steric hindrance that the atomic clusters should overcome during the rotation, it can serve as a parameter for judging the difficulty degree of a twinning mode to occur. The value of RDM in the \{10\bar{1}4\} twinning (0.845\alpha) is remarkably larger than that in \{10\bar{1}2\} twinning (0.349\alpha), \{10\bar{1}1\} twinning (0.517\alpha) and \{10\bar{1}3\} twinning (0.539\alpha) as shown in Fig. 4, which is in agreement with the common experimental facts that the \{10\bar{1}4\} twinning has almost never been found. The discovery of the GACs induced mechanism in \{10\bar{1}4\} twinning in return broadens the applicability of this mechanism in the HCP crystals.

4. Conclusion

The law of atomic motion in \{10\bar{1}4\} twinning is revealed by using the GACs rotation model. It is found that the GACs in \{10\bar{1}4\} twinning rotate by an angle of 20.2° without making a shifting along the longitudinal direction of the clusters. As an important parameter to judge the difficulty degree of twinning to occur, the value of the RDM in \{10\bar{1}4\} twinning (0.845\alpha) is significantly larger than that in \{10\bar{1}2\}, \{10\bar{1}1\} and \{10\bar{1}3\} twinning, which is consistent with the fact that the frequency of the occurrence of this twinning mode is much lower than the others.

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