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An explanation for the formation of polyhedral abnormal grains in single-phase systems

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Morphologically distinctive grain boundaries, present in a model Ni system with cube-shaped abnormal grains, were characterized via transmission electron microscopy. It is revealed that the boundaries terminated by {100} planes are energetically and kinetically more stable than other boundaries terminated by other planes. These findings indicate that abnormal grains assume a polyhedral shape when specific planes are highly singular and their migration is governed by step formation and growth, irrespective of the orientation of matrix grains.

Keywords: Abnormal grain growth; Ultrafine Ni; Grain boundary migration; Faceting; Singular

When abnormal grain growth (AGG) occurs in a single-phase system, abnormal grains often take the form of well-faceted polyhedra, as observed in $BaTiO_3$ [1–5], Al_2O_3 [6,7] and Ni [8–11]. In addition, this shape is usually maintained during their growth. The maintenance of the polyhedral shape implies that the velocities of the migrating boundaries are conserved, irrespective of the orientations of the adjacent shrinking matrix grains, and the facet planes have the lowest migration velocities. The planar boundaries are usually terminated and conserved by low-index planes during abnormal growth, e.g. {111} planes in $BaTiO_3$ [3–5], {0001} planes in Al_2O_3 [7] and {100} planes in Ni [11].

According to the classical theory of grain boundary migration [12], the migration velocity, v_b, is expressed as:

$$v = M_b \gamma_b K, \quad (1)$$

where M_b is the grain boundary mobility, γ_b is the grain boundary energy and K is the average curvature of the boundary. As each boundary between a large abnormal grain and a small matrix grain is believed to have different mobility [13] and boundary energy [14], the observation that all the different boundaries move together with the same velocity, maintaining a planar shape with a single crystallographic orientation, is puzzling.

The maintenance of a planar boundary is not readily understandable from a thermodynamic point of view. For the cube shape of abnormal grains in ultrafine-grained (UFG) Ni, it could be speculated that the shape is a result of minimization of the boundary energy of the abnormal grain. This explanation may, however, be inappropriate for a solid-state single-phase system, because the boundary energy between a growing abnormal grain and a shrinking matrix grain varies from matrix grain to matrix. In addition, the planar shape of the boundary implies that the dihedral angle at a triple junction is 180°. This is difficult to understand when considering the boundary tension balance at the triple junction.

In an attempt to understand the formation and migration behavior of planar boundaries, we observed and characterized the boundaries of abnormal grains formed in a model system of UFG Ni. Samples were prepared from ultrafine Ni powder (99.9 wt.% purity, 180 nm size, JFE Mineral Ltd., Tokyo, Japan). Cold isostatically compressed powder compacts were sintered at 550 °C in wet H_2 for various periods of time from 60 to 6000 min. Microstructures in the central region of the sintered samples were observed under a scanning electron microscope and a transmission electron

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microscope. The details of the experimental procedure are described in our previous publication [11].

After sintering ultrafine Ni powder compacts, various boundary shapes of abnormal grains were observed, as shown in Figure 1. During the growth of an abnormal grain, the boundaries are flat (Fig. 1c), but they become mostly curved (arrows in Fig. 1d) or wavy (dotted arrows in Fig. 1d) upon encountering another abnormal grain. During extended annealing of the sample after impingement of abnormal grains, practically no grain growth occurred (from 34.5 μm at 600 min sintering to 36.8 mm at 6000 min sintering), but the curved and wavy shapes of impinged boundaries largely changed into well-faceted angular boundaries, as shown in Figure 1b (circles) and e.

Considering the curved or wavy boundary shapes that arise immediately after impingement, the boundary area appears to increase with the shape change into a well-faceted angular shape. This indicates that the faceted angular shape (Fig. 1e) is a lower-energy configuration than the curved or wavy shape (Fig. 1d). As the misorientation relation between two impinged grains is unchanged during extended sintering, this energetic accommodation of the boundary must be achieved by changing its boundary plane, revealing the presence of energetic singularities of the boundary plane in this system.

Figure 2a shows a typical bright-field transmission electron microscopy (TEM) micrograph of migrating boundaries observed along the [001] zone axis of an abnormal grain. The average normal direction of the migrating boundaries of the abnormal grain is [100], although the exact normal direction of the boundaries slightly deviates from [100], as shown in Figure 2a. The atomic structure of the migrating boundary in Figure 2b, however, shows that the boundary consists of many ordered (100) planes of abnormal grain and connecting steps. This boundary configuration was confirmed for more than 10 straight migrating boundaries,

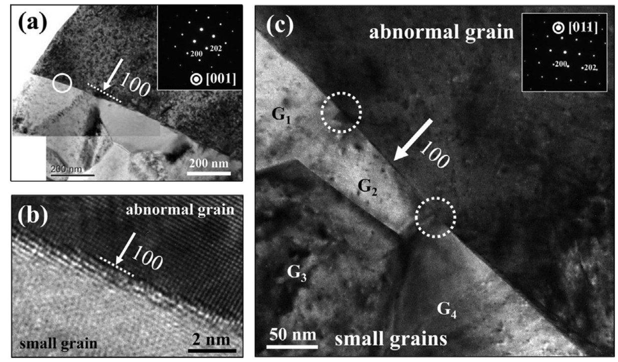

Figure 2. (a) Bright-field TEM micrograph of boundaries between an abnormal grain and matrix grains and (b) high-resolution TEM micrograph of a boundary (circle) in (a) in a sample sintered at 550 °C for 60 min. (c) Bright-field TEM micrograph showing triple junctions in the same sample.

which were also observed along the <001> zone axis of the abnormal grains. This finding shows that the cube shape of abnormal grains in UFG Ni consists of {100} planes.

The straightness of the migrating boundaries with {100} planes was also maintained even at triple junctions, with an apparent dihedral angle of 180°, as indicated in Figure 2c with dotted circles. The maintenance of the straight boundary during its migration indicates that the torque for rotating the boundaries to an energetically favorable plane dominates their equilibria at the triple junction [7].

Curved and wavy impinged boundaries were also observed by TEM for more than 50 different regions. Figure 3a shows an example of curved impinged boundaries. When two abnormal grains with {100} planes meet each other and grow, the trace of contact between the two growing grains must be curved because the point of contact is impinged with a drastic reduction in the local driving force for migration. The atomic structure

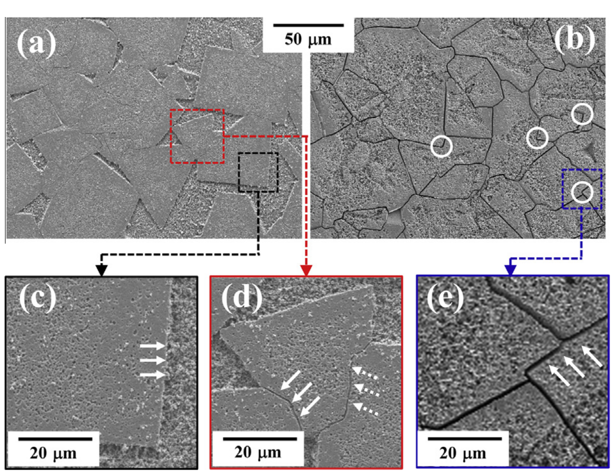

Figure 1. SEM micrographs showing the microstructures of UFG Ni samples sintered at 550 °C in wet-H_2 for (a) 60 min and (b) 6,000 min. Enlarged micrographs showing the shapes of (c) straight migrating boundaries of an abnormal grain, (d) curved (indicated by arrows) and wavy (indicated by dotted arrows) impinged boundaries, and (e) angular impinged boundaries.

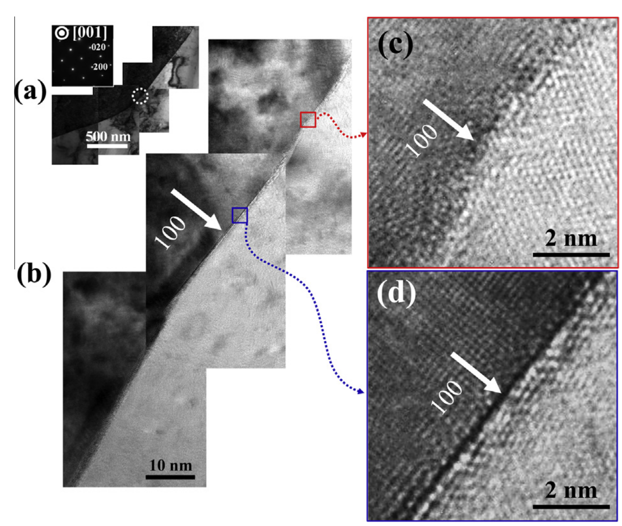

Figure 3. (a) Bright-field and (b) high-resolution TEM micrographs showing a curved impinged boundary between two abnormal grains in a sample sintered at 550 °C for 60 min. The curved boundary consists of (d) an ordered (100) plane and (c) a disordered segment.