PROCEEDINGS OF THE INTERNATIONAL CONFERENCE NANOMATERIALS: APPLICATIONS AND PROPERTIES
Vol. **1** No 3, 03PCSI01(4pp) (2012)

Kinetic Properties of the First Order Ridges in Zn

V.G. Sursaeva[*]

Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, 142432 Moscow District, Russia

(Received 21 May 2012; published online17 August 2012)

The migration of a grain boundary system with ridges of the first order is studied. A theory of steady-state motion of a grain boundary (GB) half-loop with facets and ridges is presented. The shape and properties of a moving grain boundary which contains additional structural elements (curved segments, facets and ridges of first order) are addressed. The major kinetic parameters (mobility and its activation enthalpy) of the "high-temperature" and "low-temperature" grain boundary ridge of first order with curved segments were measured.

Keywords: Grain boundary, Grain boundary of first order ridge, Migration, zinc.

PACS numbers: 61.05. – a, 61.72.Cc, 61.72.Ff, 64.70.K –

1. INTODUCTION

Grain boundaries, grain boundary triple junctions, grain boundary facets and ridges appear as the nanoobjects because of values of these structure defect width are order of 10^{-9} m. Traditionally, grain growth in polycrystals is solely attributed to the motion of grain boundaries. With growing interest in fine grained and even nanocrystalline materials also the need arose to consider the role of other structural grain boundary elements: facets, triple junctions[1-15].

In particular, it was shown that the kinetics of grain boundary triple junctions may be different from the kinetics of the adjoining grain boundaries. This affects the kinetics of microstructure evolution during grain growth, especially in fine grained materials [1-6, 13-15].

Studies of the influence of facets on the migration of a high-angle grain boundary during steady-state motion were recently reported [11, 12]. For the first time the mobility of the facets of high-angle boundary was measured in a reproducible physical experiment. A surprising result of [11, 12] was the high facet mobility with very low activation enthalpy.

However, besides the grain boundary itself, boundary triple junctions and facets, there is another kind of grain boundary structure elements, a grain boundary ridge. As early as 1951 Herring pointed out that an equilibrium shape of a crystal can contain edges and corners even though there are no flat facets [16]. The concept of grain boundary ridges was developed by Cahn and Hoffmann in 1974 [17]. They proved that two curved (rough) surfaces may intersect along a line where the boundary plane changes discontinuously. This line is called a first –order "rough-to-rough" ridge. A classification of various grain boundary ridges is given in [18].

As much as grain boundary motion can be affected by triple junctions a first order ridge may also tangibly impact the kinetics of grain boundary motion and grain growth. The major goal of the current study was to explore the formation of the "high-temperature" and "low-temperature" first order ridge and the quantitative determination of both the kinetic properties of the grain boundary system with the ridge and of the ridge itself.

2. EXPERIMENTAL

The experimental technique of the crystal manufacture was described comprehensively in [1, 16]. Flat bicrystals from 99.999 wt% Zn with a grain boundary (GB) half-loop (Fig. 1) were grown. The misorientation angle of a $\left[10\bar{1}0\right]$ tilt grain boundary half-loop is 30°. The reciprocal density of coincidence sites for the studied 30° $\left[10\bar{1}0\right]$ tilt grain boundary was $\sum = 17$. Both the flat and curved grain boundary segments were oriented perpendicular to the surface of the sample. The motion of the boundary and its shape were observed and recorded *in-situ* on the hot stage of an optical microscope in the temperature range 280-410 C using polarized light. The temperature was stable within ±0.5K during the measurement, and the temperature was increased from 280 C or decreased from 410 C for consecutive isothermal anneals by 5 or 10 K. Each isothermal anneal took 120 s or 180 s; the temperature of the hot stage and the sample stabilized in a few seconds. The annealing was carried out in the pure nitrogen atmosphere to protect the samples from oxidation. The GB shape was imaged in the course of the experiment by a video camera connected to the microscope and recorded by a VCR.

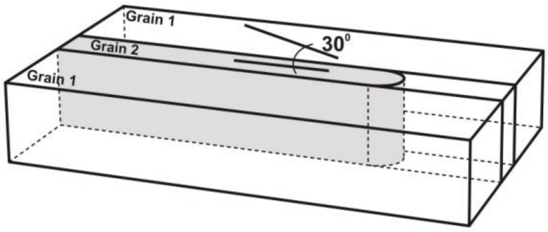

Fig. 1 – Scheme of the Zn bicrystal containing the $[10\bar{1}0]$ tilt GBs with misorientation angles of 30°. The lines denote the orientation of basal plane (0001) in both grains [11]

---

[*] sursaeva@issp.ac.ru

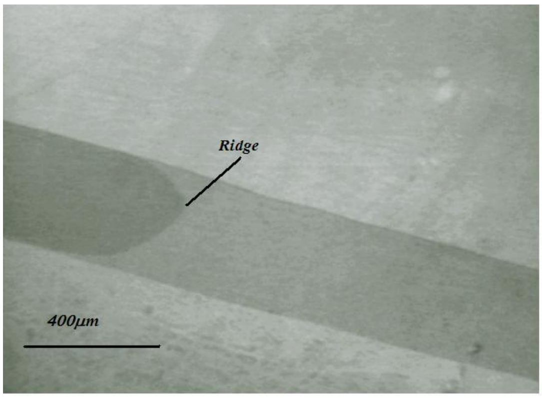

Fig. 2 – Video frame of a moving grain boundary half-loop with "high-temperature" first order ridge (T = 400 °C)

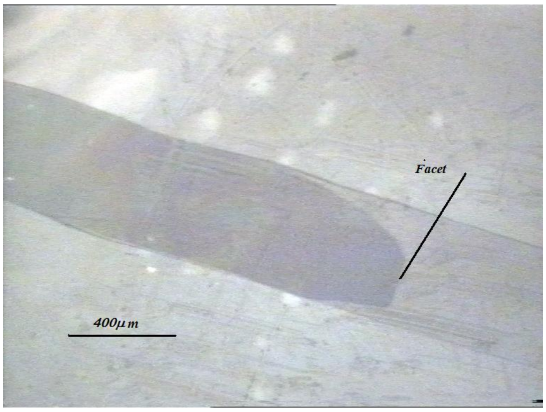

Fig. 3 – Video frame of a moving grain boundary half-loop with facet (T = 335 °C)

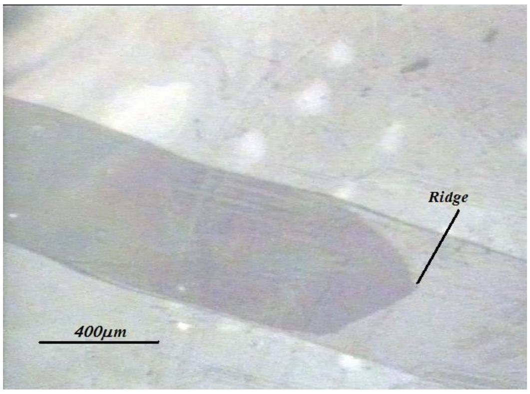

Fig. 4 – Video frame of a moving grain boundary half-loop with "low-temperature" first order ridge (T = 310 °C)

3. RESULTS

The behavior of the grain boundary system in the temperature range 280 ÷ 410 C was studied. At the temperature higher than 390 C the moving grain boundary half-loop comprised only curved segments with first order ridge (Fig. 2). Facet formation on a moving half-loop was observed during cooling (Fig. 3) at 390 C [11]. The peculiarities of grain boundary half-loop motion were reported in [11]. In particular, the steady-state character of the half-loop motion was confirmed: the rate of the half-loop migration, after some short time, when the temperature of the sample was established, was found to remain constant for both the faceted and the non-faceted grain boundary. The length of the facet was controlled by the temperature of the experiment [11]. The lowest temperature of grain boundary half-loop migration studied in [11] was 360 C. In accordance with the concepts which were outlined in [11], the length of the facet increased with decreasing temperature. However, as observed in [12], a further decrease of the temperature led to a disappearance of the facet and, surprisingly, to the formation of a new structural element – grain boundary "rough-to-rough" ridge of the first order (Figs. 4, Fig. 5) ("low-temperature" ridge).

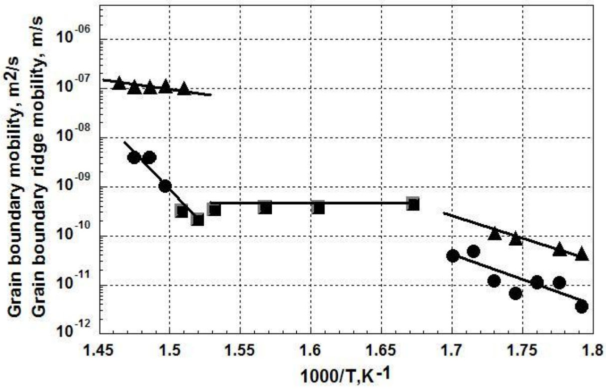

Fig. 5 – Mobility *A* of the grain boundary half-loop $A = \upsilon^{*}a[m^2/s]$ with facet (solid squares) and with ridge (solid circles and triangles).

To prove the formation of a true ridge we used the following line of arguments.

a) At a high temperature the moving grain boundary half-loop was composed of ridge with curved segments only ("high-temperature"). A reduction of the temperature caused grain boundary faceting. A further fall of the temperature led to a disappearance of the facets and the formation of a "rough-to-rough low-temperature" ridge. It is stressed that all discussed boundary transitions between the observed configurations were reversible

b) The motion of the "low-temperature" first order ridge was observed in a temperature range where the triple junction motion in Zn was never found.

c) The ridge formation changed essentially the character of motion of the grain boundary system: instead of nearly athermal motion, which was observed for the moving faceted half-loop, the half-loop with ridge demonstrated thermally activated motion with a rather large activation enthalpyergy (~2.4 eV for motion of "rough-to-rough low-temperature" ridge and ~4.9 eV for motion of "rough-to-rough low-temperature" ridge.

d) Orientation measurements by EBSD and metallographic observations did not reveal any low angle grain boundary at the ridge.

e) Finally, the microstructure of studied bicrystals in the region of the ridge was analyzed by X-ray topography (Schultz technique [19, 20]; the smallest misorientation between next neighbor grains which can be detected by this technique is 1-3 ´). The missing evidence of a misorientation at the ridge proved that the observed boundary configuration was not the consequence of a low angle boundary (at least with the misorientation larger than ~ 3´) attached to the tip of the ridge.

4. DISCUSSION

4.1 Theory of motion of a grain boundary with a ridge of first order

Let us consider the steady-state motion of a moving half-loop with a ridge of first order. (Fig.6)

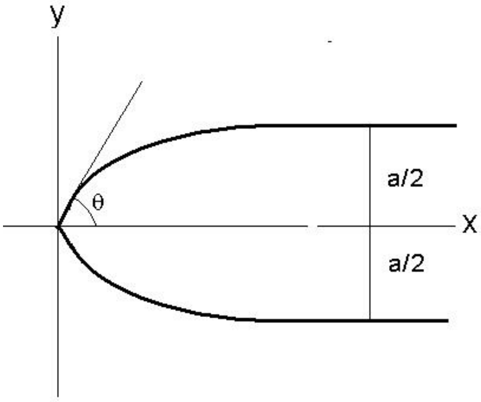

Fig. 6 – Geometry of a grain boundary half-loop with a "rough-to-rough" ridge of first order. [12]

The velocity V of the curved boundary is

$$V = 2\frac{\theta m_b \gamma_b}{a} \qquad (4.1)$$

Here, $m_b, \gamma_b\, a$ are grain boundary mobility, surface tension and grain width, respectively.

On the other hand, the velocity of the ridge migration can be described as:

$$V_r = m_r P_r \qquad (4.2)$$

where m_r is the mobility of the ridge and P_r is the driving force for ridge motion.

From Fig. 6 it can be seen that

$$P_r = 2\gamma_b \cos\theta \qquad (4.3)$$

Since for a steady-state motion the ridge and curved segments of the half-loop have to move with the same velocity, the migration rate of the grain boundary half-loop with a ridge is also controlled by the ridge motion:

$$V = V_r \qquad (4.4)$$

From Eqs. (4.1) - (4.5) we arrive at:

$$m_r = \frac{m_b \theta}{a\cos\theta} \qquad (4.5)$$

Apparently, relation (4.6) associates the angle θ with the value of the dimensionless parameter Λ_r.

$$\Lambda_r = \frac{m_r a}{m_b} = \frac{\theta}{\cos\theta} \qquad (4.6)$$

which characterizes the inhibiting influence of the ridge on grain boundary motion.

It can be seen that Eq. (4.5) matches the expectations for the limiting cases. A grain boundary ridge with large mobility m_r does not drag the motion of the grain boundary system, the angle θ tends to $\pi/2$, and the configuration transforms to the well known grain boundary half-loop where the velocity of the half-loop is determined by grain boundary mobility. For low mobile ridge the angle θ tends to zero.

Mathematical expressions are arranged directly in the text or type in a separate line, if the formula is too cumbersome or is important. In the case of existing the references to the expression further in the text, it should be numbered. The numbering of formulas can be cross-cutting across all sections or two-level, where the first level is the number of sections, and the second begins anew with each new section.

4.2 Determination of ridge mobility

Relation (4.5) makes it the possible to determine the mobility of grain boundary ridge if grain boundary mobility m_b is measured in an independent experiment [13].

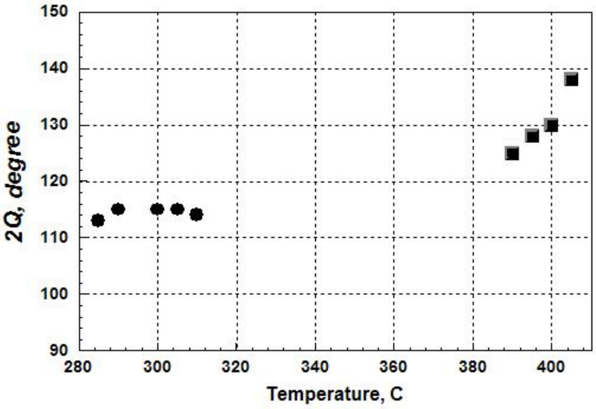

Fig. 7 – Temperature dependence of the angle 2θ at the tip of the "rough-to-rough" ridge of the first order.

The Fig. 7 demonstrates the experimentally measured temperature dependence of the angle θ between the tangents to curved boundaries at the tip of the first order ridge. On the basis of independently measured values of grain boundary mobility m_b [13] and data from the Fig. 8 the mobility of the ridge can be defined. In case when the migration of the half-loop is controlled by the motion of the ridge the kinetic parameters of the migration should be determined by the parameters of the ridge. The principal argument in favour of such a behavoiur is the parameter Λ_r. As it was shown in [12], the rather small value of the parameter Λ_r indicates that the ridge drags and at the same time controls the migration of the half-loop. In our case the parameter $\Lambda_r = 1.2 \div 1.8$ in the measured temperature range (280÷350 °C), and $\Lambda_r = 2.7 \div 3.0$ in the measured temperature range (390÷410 °C). It follows immediately that the migration of our boundary system is determined by ridge motion. In the Fig. 5 the mobility of the half-loop which is defined as the velocity V of the half-loop divided on the driving force (essentially the half-loop width), is marked by solid circles while the mobility of the ridge, defined as described above, is marked by solid triangles. The activation enthalpy of migration which is determined from half-loop motion as a whole and the ridge migration is equal to 2.4 eV and 1.1 eV accordingly for "low-temperature" ridge and to 4.9 eV and 0.1 eV accordingly for "high-temperature" ridge. The strong reduction of the major kinetic parameter, the enthalpy of activation, which derives from both the change of the angle θ with temperature and the dependency $m_r(\theta)$, points to the fact that the migration of our grain boundary system is governed by the "rough-to-rough" ridge of first order.

5. CONCLUSION

1. The steady-state migration of a special 30° $\left[10\bar{1}0\right]$ tilt grain boundary half-loop with the facets and with the ridges of the first order was studied.

2. A theory of steady-state motion of a grain boundary half-loop with ridges is presented.

3. For the first time the mobility and the activation enthalpy of migration of a "rough-to-rough" high-temperature and low-temperature grain boundary ridge of first order has been measured.

AKNOWLEDGEMENTS

We appreciate the financial support of the Russian Foundation of Fundamental Research (Grant RRFI 12-03-00894).

REFERENCES

1. Gottstein G, Shvindlerman L.S., *Grain Boundary Migration in Metals: Thermodynamics, Kinetics, Applications, 2nd edition*, (CRC Press, Boca Raton, Fl:2010).
2. Czubayko U, Sursaeva V.G, Gottstein G, Shvindlerman L.S., *Acta Mater.* **46**, 5863 (1998).
3. Gottstein G, Shvindlerman L.S., *Acta Mater.* **50,** 703 (2002).
4. Gottstein G, Ma Y, Shvindlerman L.S., *Acta Mater.* **53**, 1535 (2005).
5. Mattissen D, Molodov D.A., Shvindlerman L.S., Gottstein G., *Acta Mater.* **53**, 2049 (2005).
6. Protasova S.G., Gottstein. G, Molodov D.A., Sursaeva V.G., Shvindlerman L.S., *Acta Mater.* **49**, 2519 (2001).
7. Hsieh T.E., Balluffi R.W., *Acta Metall.* **37**, 2133 (1989).
8. Watson G.M., Gibbs D., Song S., Sandy A.R., Mochril S.G.J., Zener D.M., *Phys. Rev.* **52**, 12329 (1995).
9. Lee S.B., Yoon D.Y., Henry M.B., *Acta Mater.* **48**, 3071 (2000).
10. Rabkin E.J., *Mat. Sci.* **40**, 875 (2005).
11. Sursaeva V.G., Straumal B.B., Gornakova A.S., Shvindlerman L.S., Gottstein G., *Acta Mater.* **56**, 2728 (2008).
12. V.G. Sursaeva, G. Gottstein. L.S. Shvindlerman, *Acta Mater.* **41**, 7725 (2010).
13. A.V. Antonov, Kopetskii Ch.V., Shvindlerman L.S., Sursaeva V.G., *Sov. Phys. Dokl.* **18**, 736 (1974).
14. Gottstein G, Shvindlerman L.S., Sursaeva V.G., *Int. J. Mat. Res.* **52**, 491 (2008).
15. Barrales-Mora L.A., Shvindlerman L.S., Mohles V., Gottstein G., *Mat. Sci. Forum* **558**, 1051 (2007).
16. Barrales-Mora L.A., Shvindlerman L.S., Mohles V., Gottstein G., *Acta Mater.* **56**, 1151(2008).
17. Barrales-Mora L.A., Gottstein G., Shvindlerman L.S., *Acta Mater.* **56**, 5915 (2008).
18. Herring C., *Phys.Rev.*, **82**, 87 (1951).
19. Cahn J.W., Hoffman D.W., *Acta Metall.* **22**, 1205 (1974).
20. Straumal B.B., Sursaeva V.G., Baretzky B., *Scripta Mater.* **62**, 924 (2010).
21. Schulz L.G., *J. Metals*, **6**, 1082 (1954).
22. Aristov V.V., Shulakov E.V., *J. Appl. Crystallogr.* **8**, 445 (1975).