
Volume 62, issue 12, June 2010
ISSN 1359-6462
ELSEVIER
Scripta MATERIALIA
A LETTERS JOURNAL
STRUCTURE
PROPERTIES
THEORY
PROCESSING
FUNCTION
VIEWPOINT SET
Triple Lines
Guest Editor: Andreas Mortensen
Available online at ScienceDirect www.sciencedirect.com
www.elsevier.com/locate/scriptamat

Available online at www.sciencedirect.com
ScienceDirect
Scripta Materialia 62 (2010) 924–927
Scripta MATERIALIA
www.elsevier.com/locate/scriptamat

Viewpoint Paper

Grain boundary ridges and triple lines

B.B. Straumal,[a,b,*] V.G. Sursaeva[a] and B. Baretzky[b,c]

[a]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka 142432, Russia
[b]Max-Planck Institut für Metallforschung, Heisenbergstraße 3, 70569 Stuttgart, Germany
[c]Karlsruhe Institute of Technology, Institute for Nanotechnology, Herman-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Germany

Received 22 January 2010; accepted 6 February 2010
Available online 10 February 2010

Abstract—The classification of various grain boundary (GB) and surface triple lines is given. The observations of "degenerated" GB triple lines, like first-order and second-order facet-to-facet, rough-to-facet and rough-to-rough ridges, are discussed, together with their influences on the GB mobility. Some interesting phenomena remain undisclosed by experiments and should be studied in the future.

Keywords: Grain boundaries; Triple lines; Ridges; Facets; Roughening

This issue of *Scripta Materialia* is devoted to the triple lines in materials. Most commonly known are the triple lines at the intersection of three different phases (e.g. solid, liquid and vapor phases; see the scheme in Fig. 1a). When the number of contacting phases decreases to two, we can consider another, "degenerated", triple line at the intersection of a grain boundary (GB) in a solid phase with an interphase boundary (solid/solid, solid/liquid or solid/vapor) (Fig. 1b). If a second solid phase in such a triple line is the same as the first one, our object degenerates again, and we obtain the triple junction of three similar or different GBs (Fig. 1b). However, the degeneration of a triple line can continue further. Two different kinds of GBs exist in solids, namely high-angle and low-angle GBs. If the misorientation angle θ of a GB is above $\sim 15°$, the GB is a continuous two-dimensional defect with a thickness of 1–2 lattice spacings. If $\theta < 15°$, the GB consists of an array or grid of one-dimensional defects, namely lattice dislocations. Between the dislocations, the lattice of one grain continuously transforms into the lattice of a second grain. As $\theta \to 0°$, the distance between lattice dislocations converges to infinity. At $\theta = 0°$ we obtain the next case, namely the first-order GB ridge at the intersection of two flat GB facets (Fig. 1e). "First-order" means that if we consider the GB facets as the surface (or GB) phases, the first derivative $\partial y/\partial x$ has a break at the intersection line of both GB portions. A first-order GB ridge can also appear at the intersection of a flat GB facet with a rough GB portion (Fig. 1f). If the first derivative $\partial y/\partial x$ has no break and the transition from a facet into rough GB is continuous, we obtain a second-order GB ridge (Fig. 1g). Figure 1h demonstrates the last and most exotic object in the "degeneration raw", the first-order ridge at the intersection of two rough GB portions. In this paper the unusual degenerated triple lines (Fig. 1d–h) are discussed.

The sharp GB ridges between two GB facets (first-order facet-to-facet ridges, Fig. 1e) can be observed in the case of coincidence or near-coincidence GBs. Good examples are the twin GBs in various metals, especially in those with a face-centered cubic lattice (fcc). In metals with a cubic lattice, twin GBs are also $\Sigma 3$ GBs. Their structure can be described by the coincidence sites lattice (CSL) [1] where each third atomic site of lattice 1 coincides with a site in lattice 2. The facet planes are usually parallel to the most closely packed CSL planes. With increasing temperature, GB facets become unstable due to the faceting–roughening transformation at certain T_R. The faceting–roughening transformation was first predicted and observed for free surfaces [2–7]. With decreasing temperature, the facets along less and less closely packed CSL planes consequently become stable and appear in the microstructure [8]. A similar

---

* Corresponding author. Address: Institute of Solid State Physics, Russian Academy of Sciences, Laboratory of Interfaces in Metals, Instituskaja St. 2, Chernogolovka 142432, Russia. Tel.: +7 4965 222957; fax: +7 4992382326; e-mail addresses: straumal@issp.ac.ru, straumal@mf.mpg.de

1359-6462/$ - see front matter © 2010 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.
doi:10.1016/j.scriptamat.2010.02.018

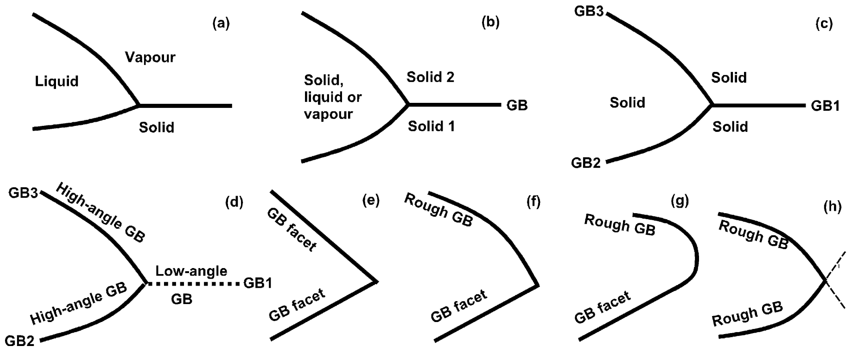

Figure 1. Scheme of sequentional degeneration of triple lines (sections perpendicular to the triple lines). (a) Contact between solid, liquid and gaseous phases. (b) The intersection line of a grain boundary in solid phase and interphase boundary between solid 1 and solid 2, or the liquid or gaseous phase. (c) GB triple junction, i.e., the intersection line of different high-angle GBs: GB1, GB2 and GB3. (d) GB triple junction, i.e., the intersection line of two high-angle GBs (GB2 and GB3) and a low-angle one (GB1). (e) First-order GB ridge at the interception of two flat GB facets. (f) First-order GB ridge at the intersection of a flat GB facet and a rough GB. (g) Second-order GB ridge at the intersection of a flat GB facet and a rough GB. (h) First-order ridge at the intersection of two rough GB portions (tangents to both portions are shown by thin dotted lines).

phenomenon was first observed at free surfaces [9]. In metals with low stacking-fault energy, like Cu, first-order facet-to-facet ridges (Fig. 1e) appear more frequently [8,10–13]. The same $\Sigma3$ GBs in Al (being a metal with a high stacking-fault energy) have much fewer facets in comparison with Cu [14–16].

In the exact $\Sigma3$ GBs in Cu only first-order facet-to-facet ridges (Fig. 1e) are present. First-order facet-to-rough ridges (Fig. 1f) appear if the misorientation angle deviates from the exact CSL value [10,14] or at high temperatures in the high stacking-fault energy metals [15]. This is because the GB faceting–roughening transformation proceeds with increasing temperature and/or increasing deviation from the exact CSL misorientation [17,18].

Second-order facet-to-rough GB ridges (Fig. 1g) have never been observed in fcc metals, to the best of our knowledge. Second-order facet-to-rough surface ridges were first observed and analyzed for Pb surfaces [7,19–22]. Similar second-order GB ridges were later observed in $\Sigma3$ GBs in Mo [23] and then in Nb [24]. Both metals have a less closely packed base-centered cubic lattice and a high stacking-fault energy. The surface or GB shape near the second-order facet-to-rough ridge can be described by the scaling theories of Andreev [25] and Pokrovsky and Talapov [26]. Using quantitative analysis of the surface or GB shape, one can calculate the so-called critical index β and decide which model is more suitable – that of Andreev ($\beta = 2$) or that of Pokrovsky and Talapov ($\beta = 3/2$) [7,23,24,27].

The first-order rough-to-rough GB ridges (Fig. 1h) are the most unexpected ones: two curved surfaces or GBs intersect and form a sharp ridge. We found such ridges for the first time in the tubular $\Sigma3$ GB in Mo [23]. The first thought of anyone who observes such a ridge in the microstructure is that it is just a GB triple joint (Fig. 1d) where one of the GBs has a low misorientation angle and therefore, is not visible after simple etching. However, we carefully studied the rough-to-rough ridges in the tubular $\Sigma3$ GB in Mo with the aid of electron-backscattering diffraction and did not find any low-angle GB contacting the ridge (at least with $\theta > 2^\circ$) [23].

Triple lines, facets and various ridges greatly influence the GB mobility [27–35]. The in situ experiments with the GBs in Zn bi- and tricrystals permitted us to measure the GB mobility and to observe the changing GB shape simultaneously, in the same experiment. We were able to do this because Zn has a non-cubic lattice and possesses optical anisotropy, allowing to analyze the GB shape under polarized light. It was possible to observe that (i) different facets of the same GB have extremely different mobilities [28,29]; (ii) a GB with a facet migrates at least one order of magnitude slower than the same GB without a facet [30,31,33]; (iii) the length of a GB facet decreases with increasing temperature due to the roughening transition [32,34]; and (iv) first-order facet-to-facet ridges (Fig. 1e) transform with increasing temperature into two second-order facet-to-rough ridges (Fig. 1f) [27].

It was most exciting to observe how two first-order facet-to-rough ridges separated by a GB facet (Fig. 2a) merged together with increasing temperature and form a first-order rough-to-rough GB ridge (Fig. 2b). This phenomenon was observed using the Zn $[10\bar{1}0]$ flat bicrystal grown from Zn of 99.999 wt.% purity using a modified Bridgman technique. It had a tilt GB with $\theta = 30^\circ$. Two flat portions of a 30° GB grew parallel to one another, forming a loop at one point (Fig. 2). Both flat and curved GB parts were perpendicular to the surface of the sample. The $[10\bar{1}0]$ axes in both grains were also perpendicular to the surface of the sample. The GB loop moved under a constant capillary driving force determined by the width of the middle grain. The shape of the migrating GB loop was studied in the temperature range between 633 and 683 K in situ in the hot stage of a light microscope using polarized light. The temperature was stabilized with an error of ± 0.5 K. The temperature steps between isothermal anneals were 5 or 10 K. The duration of the isothermal anneals was 120 or 180 s, and the "new" temperature of the hot stage and sample stabilized within a few seconds. The samples were protected from oxidation by a high-purity (99.999%) nitrogen atmosphere.

In Figure 2c the evolution of the shape of the moving GB loop is shown schematically. At low temperatures a

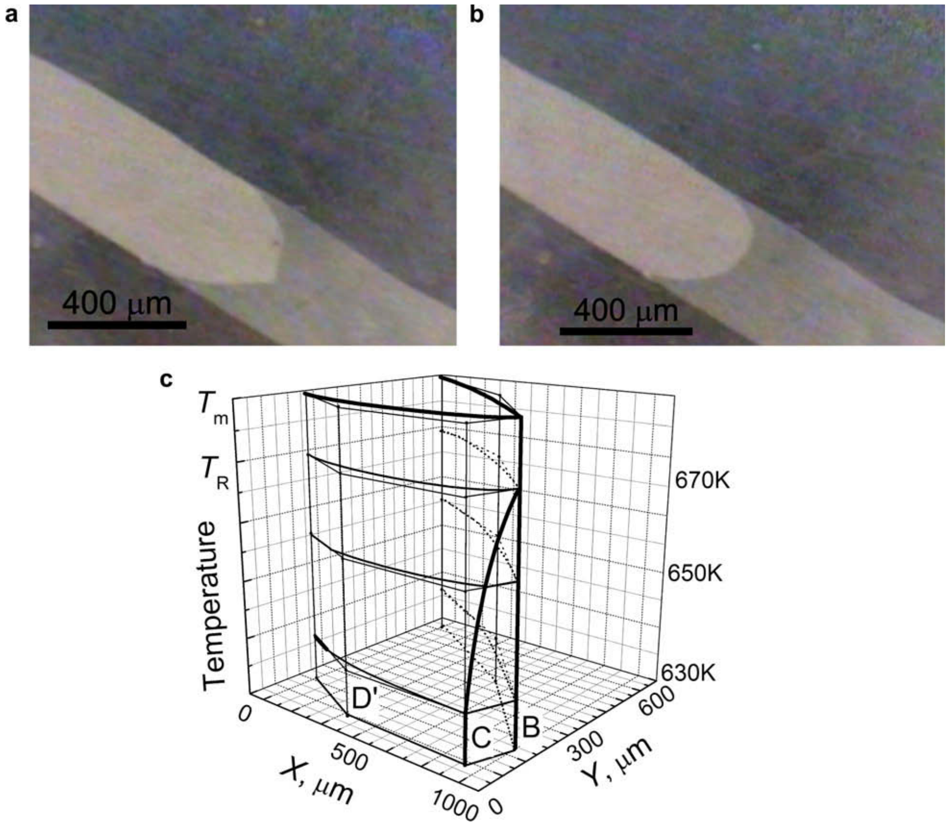

Figure 2. Optical micrographs of 30° $[10\bar{1}0]$ tilt GB. (a) The long facet and two first-order facet-to-rough ridges, $T = 643$ K (below T_R). (b) The first-order rough-to-rough ridge, $T = 678$ K (above T_R). The short facet and two first-order facet-to-rough ridges, $T = 673$ K. (c) Scheme of the influence of temperature on the shape of the GB loop with a facet between two first-order facet-to-rough ridges at temperatures below T_R and with a first-order rough-to-rough ridge above T_R.

GB loop has a facet dividing two first-order facet-to-rough ridges. This facet is parallel to the closely packed plane of a constrained coincidence sites lattice (CCSL) for the 30° $[10\bar{1}0]$. The *c*/*a* value is irrational in Zn, *a* being the lattice spacing in the basal plane (0 0 0 1) and *c* being the lattice spacing in the direction perpendicular to the (0 0 0 1) plane. Therefore, the exact CSL exists in Zn only for GBs with rotation around the [0 0 0 1] axis. In all other cases the so-called CCSL approach should be used [36]. It is interesting that the tangents to the rough GB portions in the points C and B (Fig. 2c) are also parallel to closely packed CCSL planes. By increasing the temperature, the facet between points C and B disappears (Fig. 2c) and a first-order rough-to-rough GB ridge forms instead of two first-order facet-to-rough GB ridges. However, the orientation of the first-order rough-to-rough GB ridge is not arbitrary. The tangents to the rough GB portions in the ridge point remain parallel to the closely packed CCSL planes.

The possible configurations of the first- and second-order surface ridges were theoretically predicted by Davidson and den Nijs [37,38]. The predicted first-order rough-to-rough ridges were first observed by us not for the free surfaces but for the GBs [23,24,32]. However, several interesting objects and phenomena predicted by Davidson and den Nijs have still not been explained experimentally [37,38]. We plan to investigate experimentally (i) the end point of the first-order rough-to-rough ridge on the rough surface (or GB); (ii) the first- to second-order transition point on the ridge line; and (iii) the bifurcation of a first-order ridge into two second-order ridges etc.

Acknowledgments

We thank the Russian Foundation for Basic Research (contract 09-02-90469) and the Ukrainian Fundamental Research State Fund (Grant Ф28.2107) for financial support. We cordially thank Prof. E. Rabkin, Dr. A. Gornakova and Dr. S. Protasova for stimulating discussions, and Mr. A. Nekrasov for the help with SEM and EPMA measurements.

[1] H. Grimmer, W. Bollmann, D.T. Warrington, Acta Cryst. A 30 (1974) 197.
[2] C. Rottman, M. Wortis, Phys. Rep. 103 (1984) 59.
[3] J.C. Heyraud, J.J. Métois, J. Cryst. Growth 82 (1987) 269.
[4] T. Ohachi, I. Taniguchi, J. Cryst. Growth 65 (1983) 84.
[5] L.A.M.J. Jetten, H.J. Human, P. Bennema, J.P. van der Eerden, J. Cryst. Growth 68 (1984) 503.
[6] Y. Carmi, S.G. Lipson, E. Polturak, Phys. Rev. B 36 (1987) 1894.
[7] C. Rottman, M. Wortis, J.C. Heyraud, J.J. Métois, Phys. Rev. Lett. 52 (1984) 1009.
[8] B.B. Straumal, S.A. Polyakov, E.J. Mittemeijer, Acta Mater. 54 (2006) 167.
[9] K.O. Keshishev, A.Ya. Parshin, A.V. Babkin, Sov. Phys. JETP 53 (1981) 362.

[10] B. Straumal, S. Polyakov, E. Bischoff, E. Mittemeijer, Zt. Metallkd. 95 (2004) 939.

[11] B.B. Straumal, S.A. Polyakov, E. Bischoff, W. Gust, B. Baretzky, Acta Mater. 53 (2005) 247.

[12] Ya.V. Kucherinenko, S.G. Protasova, B.B. Straumal, Def. Diff. Forum 237–240 (2005) 584.

[13] B.B. Straumal, S.A. Polyakov, L.-S. Chang, E.J. Mittemeijer, Int. J. Mater. Res. (Zt. Metallkd.) 98 (2007) 451.

[14] O. Kogtenkova, B. Straumal, S. Protasova, S. Tsurekawa, T. Watanabe, Zt. Metallkd. 96 (2005) 216.

[15] O.A. Kogtenkova, B.B. Straumal, S.G. Protasova, P. Zięba, Def. Diff. Forum 237–240 (2005) 603.

[16] S.G. Protasova, O.A. Kogtenkova, B.B. Straumal, Mater. Sci. Forum 558–559 (2007) 949.

[17] B.B. Straumal, L.S. Shvindlerman, Acta Metall. 33 (1985) 1735.

[18] T.E. Hsieh, R.W. Balluffi, Acta Metall. 37 (1989) 2133.

[19] S. Surnev, K. Arenhold, P. Coenen, B. Voigtlander, H.P. Bonzel, P. Wynblatt, J. Vac. Sci. Technol. A 16 (1998) 1059.

[20] K. Arenhold, S. Surnev, P. Coenen, H.P. Bonzel, P. Wynblatt, Surf. Sci. 417 (1998) L1160.

[21] K. Arenhold, S. Surnev, H.P. Bonzel, P. Wynblatt, Surf. Sci. 424 (1999) 271.

[22] H.P. Bonzel, A. Emundts, Phys. Rev. Lett. 84 (2000) 5804.

[23] B.B. Straumal, V.N. Semenov, O.A. Kogtenkova, T. Watanabe, Phys. Rev. Lett. 192 (2004) 196101.

[24] B.B. Straumal, V.N. Semenov, A.S. Khruzhcheva, T. Watanabe, J. Mater. Sci. 40 (2005) 871.

[25] A.F. Andreev, Sov. Phys. JETP 53 (1981) 1063.

[26] V.L. Pokrovsky, A.L. Talapov, Phys. Rev. Lett. 42 (1979) 65.

[27] B.B. Straumal, A.S. Gornakova, V.G. Sursaeva, V.P. Yashnikov, Int. J. Mater. Res. (Zt. Metallkd.) 100 (2009) 525.

[28] B.B. Straumal, E. Rabkin, V.G. Sursaeva, A.S. Gornakova, Zt. Metallkd. 96 (2005) 161.

[29] V.G. Sursaeva, B.B. Straumal, Mat.-Wiss. U. Werkstofftech. 36 (2005) 528.

[30] B.B. Straumal, V.G. Sursaeva, A.S. Gornakova, Zt. Metallkd. 96 (2005) 1147.

[31] V.G. Sursaeva, B.B. Straumal, Def. Diff. Forum 249 (2006) 183.

[32] B.B. Straumal, A.S. Gornakova, V.G. Sursaeva, Phil. Mag. Lett. 88 (2008) 27.

[33] V.G. Sursaeva, A.S. Gornakova, V.P. Yashnikov, B.B. Straumal, J. Mater. Sci. 43 (2008) 3860.

[34] V.G. Sursaeva, B.B. Straumal, A.S. Gornakova, L.S. Shvindlerman, G. Gottstein, Acta Mater. 56 (2008) 2726.

[35] B.B. Straumal, A.S. Gornakova, V.G. Sursaeva, Crystallogr. Rep. 54 (2009) 1123.

[36] G.A. Bruggeman, G.H. Bishop, W.H. Hartt, in: Hsun Hu (Ed.), The Nature and Behaviour of Grain Boundaries, Plenum, New York, London, 1972, pp. 71–92.

[37] D. Davidson, M. den Nijs, Phys. Rev. E 59 (2000) 5029.

[38] D. Davidson, M. den Nijs, Phys. Rev. Lett. 84 (2000) 326.