ARCHIVES OF METALLURGY AND MATERIALS
Volume 51 2006 Issue 2

K. PIEŁA*

ANALYSIS OF GEOMETRICAL AND STRUCTURAL FACTORS DETERMINING PLASTIC FLOW OF TWINS IN ZINC CRYSTALS

ANALIZA CZYNNIKÓW GEOMETRYCZNYCH I STRUKTURALNYCH WARUNKUJĄCYCH PLASTYCZNE PŁYNIĘCIE BLIŹNIAKÓW W KRYSZTAŁACH CYNKU

The analysis of the geometry of twinning in zinc, the influence of the initial orientation of crystals (from the lines: [0001]–$[11\bar{2}0]$ and [0001]–$[10\bar{1}0]$ of the standard triangle) on the value of Schmid factor for twinning systems and the geometrical and structural conditions for basal slip activity in twinned areas are presented. It has been found that: i) only in the case of (tensiled) crystals with orientation close to $[11\bar{2}0]$ twinning leads to the increase of the Schmid factor for the basal system, and such mode of slip can be theoretically accompanied by the effect of 'geometrical softening'; ii) the 'latent hardening' of twins, resulting from the twinning transformation of the matrix dislocation structure, suppresses (or at least make difficult) the basal slip at low temperatures, and at higher ones – it stimulates the recrystallization process; iii) the effect of 'geometrical softening' of twins would be realized at medium temperatures only, when the processes of structure regeneration are controlled by 'dynamic recovery'.

W prezentowanej pracy poddano analizie geometrię bliźniakowania cynku, wpływ orientacji początkowej (z linii [0001]–$[11\bar{2}0]$ oraz [0001]–$[10\bar{1}0]$) na czynnik Schmida dla systemów bliźniakowania oraz warunki geometryczne i strukturalne aktywizacji poślizgu w podstawie w obszarach zbliźniaczonych. Stwierdzono, że: i) jedynie w przypadku (rozciąganych) kryształów cynku o orientacji bliskiej $[11\bar{2}0]$, zbliźniaczenie prowadzi do wzrostu czynnika Schmida w systemie podstawy, a poślizgowi w tym systemie może teoretyczne towarzyszyć efekt 'mięknięcia geometrycznego'; ii) 'umocnienie utajone' bliźniaków, będące rezultatem transformacji bliźniaczej struktury dyslokacyjnej matrycy, zapobiega (lub co najmniej utrudnia) aktywizacji poślizgu w podstawie w temperaturach niskich, zaś w temperaturach wysokich jest odpowiedzialne za procesy rekrystalizacji oraz iii) realizacja efektu 'geometrycznego mięknięcia' bliźniaków jest możliwa jedynie w temperaturach niezbyt wysokich, gdy procesy regeneracji struktury bliźniaków są kontrolowane przez 'dynamiczne' zdrowienie.

1. Introduction

Twinning is defined as a homogeneous movement of atoms (simple shear) which occurs in the twinning direction on the successive planes in such a mode that the lattice of the twin and that of the matrix of crystal are in exact crystallographic relation. Twinning causes:
- reorientation of the twin lattice with respect to crystal axis
- transformation of the matrix dislocation structure, and
- 'misalignement' of the tested crystal.

The latter one generates the bending moment in the crystal, and – because of the requirements of material continuity on the matrix/twin boundary (both after the twin nucleation as well as during the subsequent plastic flow) – it determines the activity of the additional deformation mechanisms in the matrix and/or in the twin. Several structural observations have shown that in zinc crystals deformed at ambient temperatures the twin is accommodated in the matrix by formation of kink bands, and by slip in the 2nd order pyramidal system $\{11\bar{2}2\}<\bar{1}\bar{1}23>$ as well as, eventually, by twinning in conjugate (or un-conjugate) systems [1, 2]. It is well known that work hardening makes the activity of these mechanisms more and more difficult; for example, the increase of the basal dislocation density by 1 order of magnitude causes at least 3-fold increase of the twinning stress [3], on the other hand, the increase of that by 2 orders of magnitude – over 4-fold increase of the starting stress necessary for slip in the 2nd order pyramidal system [4].

The question about the plastic flow of the twinned area is up to now open despite of the drastic differences

---

* DEPARTMENT OF STRUCTURE AND MECHANICS OF SOLIDS, AGH UNIVERSITY OF SCIENCE AND TECHNOLOGY, 30-059 KRAKÓW, AL. MICKIEWICZA 30, POLAND

in the mechanical behavior of tested crystals. On the one hand, twinning is regarded as the cause of cracking of many metallic materials (see for example [5, 6]), whereas, on the other hand, sometimes – as observed for zinc and cadmium crystals – the twinned areas can realize severe plastic deformation [7].

In the present paper the geometrical and the structural factors, responsible for the plastic flow of twin in zinc crystals are considered. The analysis concerns the geometry of the twinning process and the relation between some of the initial orientations of the crystals and the values of the Schmid orientation factor (SF) for twinning. Finally, the structural circumstances which suppress the activity of the basal slip in twinned areas are also discussed.

2. Geometry of twinning and its consequences

Twinning in zinc and cadmium occurs on the six $\{10\bar{1}2\}$ planes [7, 8] and the lattice geometry of both metals (the value of ratio of lattice parameters $c/a>1.633$) determines the 'polarity' of the twinning shear. This means that it occurs in the direction $[10\bar{1}\bar{1}]$ – and not in the opposite one – and causes the shortening of complete twinned crystals (by 6.68% in the case of zinc) in the direction of <c> axis; thus it has a 'compressed' character. The main consequence of 'polarity' of twinning shear is the subdivision of the standard orientation triangle into sub-regions, restricted by the great circles – the traces of the six twinning planes [9]. Each of the sub-region is characterized by:

- different sequence of activity of the twinning systems, and
- differentiation of the geometrical consequences of twinning.

These factors are of important practical meaning because the choice of a proper combination: crystal orientation/mode of loading (tensile or compression tests) is a necessary condition for the twinning process to start. The sequence of the activity of the twinning systems in each of the sub-region of the standard triangle was defined by the SF [9], however, neither the real values of these factors nor the mutual relations between them were known. Although, as it believed, the SF controls the system in which the first twin nucleates, the number of active twinning systems is determined both by the differentiation in the actual values of the orientation factors as well as by local stress state (i.e. influenced by grips, nucleation of subsequent twins, etc.).

The influence of the initial orientation of zinc crystals (from the lines: $[0001]$–$[11\bar{2}0]$ and $[0001]$–$[10\bar{1}0]$) on the SF's for six twinning systems is shown in Fig. 1. The $[0001]$ m angle χ_o (between the crystal axis and the direction $[0001]_M$, where M – matrix) at which the SF equals 0, determines the threshold value, below and above which the twinning causes the elongation and shortening of the crystal, respectively. For orientations from the line $[0001]$–$[11\bar{2}0]$ the threshold values are 47° and 51° (and 90° for $(\bar{1}102)$ and $(1\bar{1}02)$ twinning planes), whereas for those from the line $[0001]$–$[10\bar{1}0]$ there are the angles 43° and 47° (Fig. 1). It means that, from the geometrical point of view, twinning is allowed in compressed crystals with orientations lying from the vertex of the standard triangle [0001] up to the threshold value, whereas in those with the orientation from the 'bottom' of triangle – during the tensile test only.

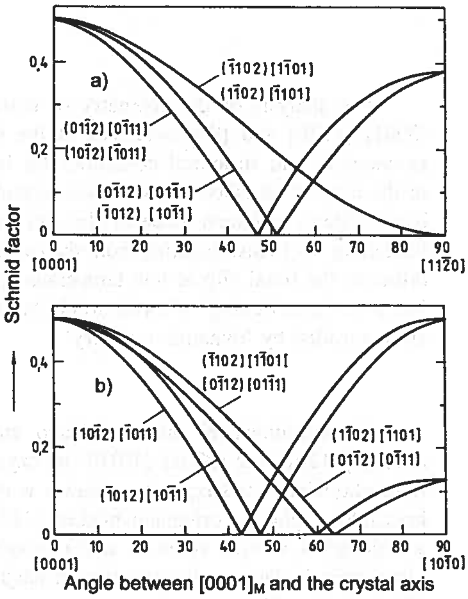

Fig. 1. The values of Schmid orientation factor for $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ twinning in zinc crystals. Orientations from the lines: a) $[0001]$–$[11\bar{2}0]$; b) $[0001]$–$[10\bar{1}0]$. (M – matrix)

For orientations close to [0001] all the six twinning systems may be active, on the other hand in crystals whose axes tend toward the directions $[11\bar{2}0]$ and $[10\bar{1}0]$ – as much as four and two systems are preferred, respectively. It is clear that in each case, the change of the loading mode makes the twinning geometrically forbidden. It is clearly seen that even a considerable deviation of orientation (for example 20°) from the directions: [0001], $[11\bar{2}0]$ and $[10\bar{1}0]$ does not essentially change the values of the SF's, i.e. it does not influence the number or the preference of the twinning systems. It is worthy of note that for the considered twinning mode, the lowering in the c/a ratio 'shifts' the values of the threshold angles only by a few degrees. For example, for beryllium, which has the lowest ratio $c/a = 1.568$, the values of χ_o are ~ 4° lower than those for zinc, but, as it known, the 'polarity' of twinning is reversed.

3. Geometrical conditions for plastic flow of twins

Twinning shear, as it was mentioned above, causes the reorientation of the lattice in the twin with respect to that in the matrix of the crystal, and also with respect to the direction of loading. Since the basal slip system is characterized by the lowest value of the critical resolved shear stress (CRSS), it is necessary to answer the questions about the influence of the initial orientation of the crystals on:

- the orientation of the basal plane in as formed twin
- the possibility and the consequences of (eventual) basal slip in the twin, and
- if necessary, show the alternative mechanisms of plastic flow of twin.

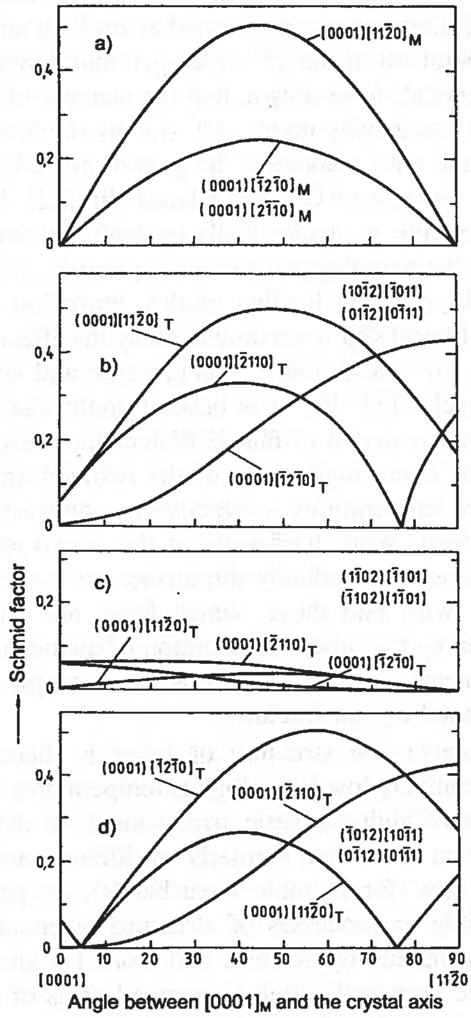

Fig. 2. The values of Schmid orientation factor for basal systems: a) in matrix (M); b-d) in twins (T). Orientations from the line $[0001]$–$[11\bar{2}0]$

The answers would indicate the conditions for occurring and the origin of the slip traces observed in twins, which are usually explained as the effect of 'geometrical softening' of the twinned area for basal slip. However, it should be remembered that such effect, if it occurs, may originate in the lattice rotation resulting from the twinning shear and/or in the subsequent basal slip.

The influence of the initial orientation of zinc crystals on the values of SF for basal systems in matrix (M) and in twin (T) is shown in Figs. 2a; 3a, and 2b-d; 3b-d, respectively. Similarly as previously, the documentation comprises the six twinning systems and the crystal orientations from the lines: $[0001]$–$[11\bar{2}0]$ and $[0001]$–$[10\bar{1}0]$. The orientations of the slip planes and slip directions in the twinned area were determined using the standard projections for zinc, according to the geometrical relation between the lattices of matrix and twin [10]. In each case the direction $<11\bar{2}0>$ (belonging to the twinning plane) was the rotation axis for both crystallographic planes and directions, and the rotation angle was 94° (two-fold of that between the basal and the twinning planes) [10].

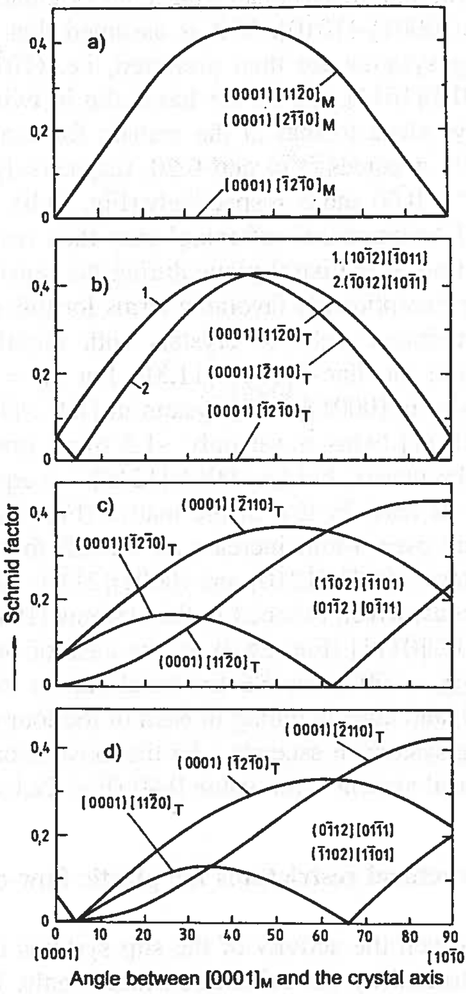

Fig. 3. The values of Schmid orientation factor for basal systems: a) in matrix (M); b-d) in twins (T). Orientations from the line $[0001]$–$[10\bar{1}0]$

Analysis of results, inserted in Figs. 2 and 3, indicates that the effect of 'geometrical softening' of twin for the basal slip can theoretically occur in the specific conditions only.

In twinned areas of crystals with the initial orientation [0001], the SF for basal system equals 0.06 and is close to that in matrix (0), and the basal plane is nearly parallel to the compression axis. Then, in such mode of loading, the small effect of 'geometrical softening' can arise at the most from the basal slip, however, the lattice rotation is rather restricted by the anvils (and by accommodation of deformation on the boundary matrix/twin). This is the case for which the activity of additional deformation mechanisms is required, and, since the basal plane in twin is nearly parallel to the crystal axis, there are these observed in compressed crystals with the orientation from the 'bottom' of the standard triangle, i.e. slip in 2nd order pyramidal system, slip in 1st order prismatic system $\{10\bar{1}0\}<11\bar{2}0>$ and kink band formation [11–13].

Similar relation between the basal slip systems in the matrix and the twin takes place for orientations from the line $[0001]–[10\bar{1}0]$. If it is assumed that only two twinning systems are then preferred, i.e. $(10\bar{1}2)[\bar{1}011]$ and $(\bar{1}012)[10\bar{1}1]$, the SF for basal slip in twin is nearly always close to that in the matrix; for example, for $\chi_o = 75^\circ$, it equals 0.26 and 0.20, respectively, and for $\chi_o = 90^\circ$ – 0.06 and 0, respectively (Fig. 3a,b). Thus, the effect of 'geometrical softening' may then results from the rotation of the basal plane during the tensile test.

The exceptionally favorable terms for this effect occur in twinned areas of crystals with initial orientations from the line $[0001]–[11\bar{2}0]$. For $\chi_o = 75^\circ$, the SF for slip in $(0001)[11\bar{2}0]$ system in $(10\bar{1}2)[\bar{1}011]$ and $(01\bar{1}2)[0\bar{1}11]$ twins is yet only ~1.5 times greater than that in the matrix, but for $(0001)[\bar{1}2\bar{1}0]$ – it equals 0.40, i.e. it is at least 3x that in the matrix (Fig. 2a,b). Similarly, the over 3-fold increase of the SF for the basal slip systems $(0001)[\bar{1}2\bar{1}0]$ and $(0001)[2\bar{1}\bar{1}0]$ takes place in the areas, which twinned in the systems $(\bar{1}012)[10\bar{1}1]$ and $(0\bar{1}12)[01\bar{1}1]$ (Fig. 2a,d). In the case of orientation $[11\bar{2}0]$ ($\chi_o = 90^\circ$), the SF for basal slip in the matrix equals 0, and after twinning in each of the four preferred twinning systems it exceeds – for the most favorably oriented basal system – the value 0.40 (Fig. 2a,b,d).

4. Structural restrictions for plastic flow of twin

However, the activity of the slip systems in twin is not controlled by the orientation factor only. It is well known that twinning results in two- and even three-fold increase of CRSS for basal slip [8, 14], and, in the opinion of Bell and Cahn [14], it origins in the conversion of the gliding dislocation in the basal and pyramidal systems in the matrix into the sessile ones in twins, the latter regarded as effective obstacles for moving dislocations. The interactions: twin/dislocation structure of the matrix and moving dislocation/twin in hexagonal lattice were numerically analysed by Yoo and Wei [15, 16] and experimentally confirmed by TEM observations (of incorporation of some types of gliding dislocations into twins) in zinc by Tomsett and Bevis [17, 18]. The results of calculations lead to the conclusion, that the only one among the three possible types of basal dislocations present in the matrix undergoes so called 'conservative' transformation to the basal one in twin. On the other hand, all remaining dislocations, i.e. both basal as well as these from the secondary systems, transform into high-energetic dislocation arrangements in twins.

It is thus clear that basal slip in the twin occurs in the conditions of 'alien' distribution of dislocations; the mechanical and structural features of such mode of plastic flow have been described for the first time in [19–21]. Experiments performed at ambient temperature on pre-strained in the 2nd order pyramidal systems zinc single crystals have shown, that the increase of the forest dislocations density up to $\sim 10^7$ (i.e. by the four order of magnitude with respect to 'as grown' crystals) leads to 20-fold increase of CRSS for basal slip [22]. Moreover, such structure is mechanically unstable; during the tensile test the twinning process takes place [6, 14, 22], and under the different loading modes, formation of coarse bands of basal slip is accompanied by the effect of 'jerky flow' or by 'yield point' (compression and shear tests, respectively) [23–26]. It is beyond doubt that the twinning transformation of matrix dislocations results in the effect of 'latent hardening' of the twinned area, which – at low temperatures – effectively suppresses the slip inside them. Work hardening of the matrix during the mechanical test gradually diminishes nucleation of successive twins and those, which form, are much more hardened by the 'alien' distribution of dislocations. As a consequence, in such conditions (for example at 293K) the twinned crystal fractures.

However, the structure of twins is thermally stable at relatively low homologous temperatures only. The presence of high-energetic arrangements of dislocations causes that the twins, similarly as different areas of localized flow (for example shear bands), are particularly susceptible to processes of structure regeneration. Yet the experiments by Schmid and Boas [7] showed that the static recrystallization in twinned areas of cadmium is much faster than that in the matrix. Moreover, it is also well known that the process of static recovery or static recrystallization drastically accelerates under external stress [29].

Under the dynamic conditions of continuous mechanical test, performed at elevated temperatures, each act of strain localization causes the division of the material into the 'temporarily' active and passive areas [30]. Inside the latter ones – as in formed twins – the dynamic (or rather 'quasi-static') processes of structure regeneration take place, and their types are controlled by the deformation temperature and strain rate (and probably by the strain). In zinc crystals with the orientation from the 'bottom' of the standard triangle, tested at high temperatures, recrystallization comprises the whole volume of the twins or the areas of twins collision only (at 573K and 473K, respectively). The lowering of the deformation temperature to 373K causes that the recrystallization diminishes and then the intensive processes of 'dynamic' recovery enable considerable plastic deformation of twinned areas (up to 'point fracture'). Plastic flow is realized by basal slip, and the rotation of the basal plane is accompanied initially by drastic drop of load, and next by load stabilization [6, 13, 31, 32]. Then, the effect of 'geometrical softening' of twins in zinc crystals can be observed when the processes of 'dynamic' recovery are sufficiently effective.

5. Conclusions

1. In the (tensiled) zinc single crystals with the orientation close to $[11\bar{2}0]$ only, the twinning leads to the increase of the value of Schmid orientation factor for basal system, and such slip mode can be theoretically associated with the effect of 'geometrical softening'.
2. 'Latent hardening' of twinned area, which originates from the transformation of the matrix dislocations, prevents the activity of basal slip at low deformation temperature, and is responsible for recrystallization process at high temperatures.
3. The effect of 'geometrical softening' of basal slip in twins in zinc crystals can be realized at medium temperatures only, when the processes of structure regeneration are controlled by 'dynamic' recovery.

Acknowledgements

The Polish State Committee for Scientific Research supported his work (grant No. 11.11.180.134).

REFERENCES

[1] P. L. Pratt, S. F. Pugh, J. Inst. Metals **80**, 653 (1951-52).

[2] H. S. Rosenbaum, Acta Met. **9**, 742 (1961).

[3] R. C. Blish, T. Jr. Vreeland, Phil Mag. **17**, 840 (1968).

[4] I. W. Getkina, F. F. Lawrentew, FMM. **41**, 1118 (1976).

[5] R. L. Bell, R. W. Cahn, J. Inst. Metals **86**, 433 (1957-58).

[6] K. Pieła, Arch. Metall. **36**, 311 (1991).

[7] E. Schmid, W. Boas, [in]: Kristallplastizität. Springer Verlag, p. 93, Berlin 1936.

[8] E. Schmid, G. Wassermann, Z. Phys. **48**, 370 (1928).

[9] F. C. Frank, N. Thompson, Acta Met. **3**, 30 (1955).

[10] P. B. Partridge, Metals and Materials **1**, 169 (1967); Met. Rev. 12 (118).

[11] K. Pieła, A. Korbel, Proc. 10th Int. Conf. Strength of Metals and Alloys (ICSMA-10), p. 167, Sendai (Japan) 1994.

[12] K. Pieła, Arch. Metall. **42**, 339 (1997).

[13] K. Pieła, Rozprawy i Monografie, z. 133. Wyd. Nauk. – Dyd. AGH. Kraków 2004.

[14] R. L. Bell, R. W. Cahn, Proc. Roy. Soc. A239, 494 (1957).

[15] M. H. Yoo, Trans. AIME. **245**, 2051 (1969).

[16] M. H. Yoo, C. T. Wei, Phil. Mag. **14**, 573 (1966).

[17] D. I. Tomsett, M. Bevis, Phil. Mag. **19**, 129 (1969).

[18] D. I. Tomsett, M. Bevis, Phil. Mag. **19**, 533 (1969).

[19] Z. S. Basinski, P. J. Jackson, Phys. Stat. Sol. **9**, 45 (1965).

[20] Z. S. Basinski, P. J. Jackson, Phys. Stat. Sol. **9**, 805 (1965).

[21] P. J. Jackson, Z. S. Basinski, Canad. J. Phys. **45**, 707 (1967).

[22] F. F. Lawrentew, [in]: Fizika deformacionnowo uprocznienia monokristałłow. Izd. Naukowa Dumka, p. 107, Kiev 1972.

[23] N. R. Risebrough, E. Teghtsoonian, Canad. J. Phys. **45**, 591 (1967).

[24] F. F. Lawrientiew, O. R. Salita, S. V. Sokolski, Phys. Stat. Sol. a 54, 145 (1979).

[25] F. F. Lawrentew, V. L. Vladymirowa, Mater. Sci. Eng. **30**, 141 (1977).

[26] F. F. Lawrientiew, V. L Vladymirowa, A. L. Gajduk, FMM. **27**, 732 (1969).

[27] J-P. Michel, G. Champier, Mater. Sci. Eng. **52**, 63 (1982).

[28] K. Pieła, Arch. Metall. **36**, 311 (1991).

[29] P. H. Thornton, R. W. Cahn, J. Inst. Metals **89**, 455 (1960-61).

[30] H. Dybiec, A. Korbel, Mat. Sci. Eng. **A117**, L31 (1989).

[31] K. Pieła, A. Korbel, Proc. JIM Int. Symp. (JIMIS-7): Aspects of high temperature deformation and fracture in crystalline materials, p. 91, Nagoya (Japan), 1993.

[32] K. Pieła, Arch. Metall. Mater. **49**, 705 (2004).

eceived: 20 September 2005.