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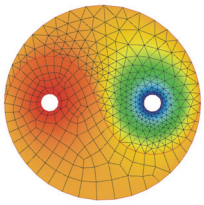

CRYSTAL PLASTICITY MODELS ACCOUNTING FOR TWINNING

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Abstract

Different approaches to account for twinning in crystal plasticity models are discussed. In particular, three main issues related to this mechanism of plastic deformation are addressed: modelling of texture evolution in the presence of twinning, impact of slip-twin interactions on hardening laws formulation and influence of layered substructure on the macroscopic response of materials. Some of the discussed modelling tools are illustrated with an example of titanium aluminide.

Key words: crystal plasticity, twinning, texture evolution, hardening

1. INTRODUCTION

Twinning mechanism is an important mechanism of plastic deformation, especially at room temperature, in the case of metals of low lattice symmetry e.g. hcp materials such as magnesium, zirconium or Ti alloys, cf. Agnew et al. (2001), Salem et al. (2005), Karaman et al. (2000), Kaschner et al. (2006), Staroselsky and Anand (2003), or intermetallics exhibiting tetragonal symmetry, cf. Mecking et al. (1996), Marketz et al. (2002), Fischer et al. (2003). In the case of these materials twinning compensates the lack of five independent slip systems required for a general shape change of volume elements enhancing metal ductility. Twinning has also a marked effect on texture development and hardening. The limited number of easy slip systems results in the development of strong crystallographic textures upon mechanical processing, e.g. rolling, cf. Agnew et al. (2001), Pospiech et al. (2006), Pospiech (2008), McCabe et al. (2009) or extrusion, cf. Wang and Huang (2007), leading to the strong anisotropy of mechanical properties of the produced components. It is particularly true for magnesium alloys, for which easy basal slip systems provide only two independent systems per grain.

As concerns fcc metals of high lattice symmetry, dislocation slip is the main mechanism of plastic deformation at room temperature for materials of medium and high stacking fault energy (sfe), e.g. copper or aluminum. However, experiments indicate, cf. Heye and Wassermann (1968), Asgari et al., (1997), El-Danaf et al. (2001), Karaman et al. (2000), that for low sfe metals (e.g. brass, MP35N alloy or Hadfield steel), the effect of mechanical twinning is significant. There exists well known issue in modelling of low sfe metals related to difference in deformation textures, especially in plane strain compression (the copper-type texture vs. the brass-type texture), as compared to high sfe metals and strong variation in the strain-stress response of materials for different deformation paths, cf. English and Chin (1965), Heye and Wassermann (1968), Asgari et al. (1997), Staroselsky and Anand (1998), Kalidindi (2001), El-Danaf et al. (2000, 2001). These facts are mainly attributed by researchers to the activity of twinning mechanism, through either the volume effect, cf. Heye and Wassermann (1968),

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Van Houtte (1978), Staroselsy and Anand (1998) or the microstructural effect, cf. Leffers and Van Houtte (1989), Leffers and Juul Jensen (1991), Leffers and Ray (2009). It should be noted that the influence of shear banding was also raised in this respect, cf. Duggan et al. (1978), El-Danaf et al. (2000), El-Danaf et al. (2001), Kalidindi (2001).

The aim of this paper is to present micromechanical modelling tools developed for the analysis of polycrystalline metals and alloys deforming by slip and twinning in the general framework of crystal plasticity theory. The following aspects are discussed in subsequent sections:

- reorientation schemes developed to model the evolution of crystallographic texture in the presence of twinning,
- the constitutive descriptions of coupling between basic inelastic deformation mechanism: slip and twinning,
- influence of a layered substructure on the macroscopic response of materials.

2. KINEMATICS AND TEXTURE EVOLUTION

2.1. Kinematics

The review is focused on the incorporation of twinning into crystal plasticity framework (Asaro, 1983), therefore the fundamental relations of the theory are not discussed. The reader is referred to the related monographs (e.g. Havner, 1992; Kocks et al., 2000). Let us only shortly summarize that for the kinematics description the multiplicative decomposition of the deformation gradient into elastic and (visco)plastic parts is used, which results in additive decomposition of the velocity gradient. Crystallographic lattice deforms only elastically and elastic stretches are small as compared to the inelastic ones, so that elastic deformations are usually neglected and only elastic rotations are taken into account leading to the texture evolution.

In classical crystal plasticity, plastic deformation occurs only by slip. The set of slip systems $\{\mathbf{n}^r, \mathbf{m}^r\}$, $r=1,\ldots,M$, depends on the lattice type (table 1).

Twinning, similarly to slip, is also realized by simple shear, with the remark that only some volume fraction of a matrix grain is sheared in the twin direction on the twin plane and with the amount of shear γ^{TW}, all specified by the lattice geometry (figure 1). Contrary to the slip mechanism, twinning is unidirectional, because due to the lattice geometry much more energy is needed to move an atom in a reverse direction (Fischer et al., 2003). The twinned sub-grain which is formed has a different, but specified lattice orientation with respect to the matrix grain (see figure 1). The crystallographic direction $\mathbf{a}^{TW}$ in the twinned part of the grain and the corresponding crystallographic direction $\mathbf{a}^{M}$ in the matrix grain are connected by the relation due to Van Houtte (1978)

$$\mathbf{a}^{TW} = \mathbf{R}^{TW}\mathbf{a}^{M} = \left(2\mathbf{n}^{TW} \otimes \mathbf{n}^{TW} - \mathbf{I}\right)\mathbf{a}^{M} \qquad (1)$$

Table 1. *The set of slip and twin systems relevant for the selected lattice symmetry (Miller indices are used and the number in brackets indicates the total number of slip/twin systems in the category considered, note that secondary twinning systems are also possible, (Kocks et al., 2000; Christian & Mahajan, 1995; Appel & Wagner, 1998).*

Lattice symmetry	Slip systems	Twin systems
fcc	{111}<1$\bar{1}$0> (12)	{111}<2$\bar{1}$1> (12) $\gamma^{TW} = 1/\sqrt{2}$
hcp	basal (0001)<1$\bar{1}$20> (3) prismatic {1$\bar{1}$00}<1$\bar{1}$20> (3) pyramidal <*a*> {$\bar{1}$101}<1$\bar{1}$20> (6) pyramidal I <*c*+*a*> {10$\bar{1}$1}<1$\bar{1}$23> (12) pyramidal II <*c*+*a*> {11$\bar{2}$2}<1$\bar{1}$23> (6)	compressive twins (for $c/a > \sqrt{3}$) {10$\bar{1}$2}<10$\bar{1}$1> (6) $\gamma^{TW} = \left\lvert\sqrt{3}/(c/a) - (c/a)/\sqrt{3}\right\rvert$ tensile twins (for $c/a < \sqrt{3}$) {10$\bar{1}$2}<10$\bar{1}$1> (6) $\gamma^{TW} = \left\lvert\sqrt{3}/(c/a) - (c/a)/\sqrt{3}\right\rvert$
fcc-like ($L1_0$, e.g. γ-TiAl)	ordinary dislocations {111}<$\bar{1}$10] (4) super-dislocations {111}<10$\bar{1}$] (8)	{111}<1$\bar{1}$2] (4) $\gamma^{TW} = 1/\sqrt{2}$

where $\mathbf{n}^{TW}$ is a unit vector normal to the twinned plane. The tensor $\mathbf{R}^{TW}$ describes the rotation around $\mathbf{n}^{TW}$ by the angle π. Tensor $\mathbf{I}$ is the second order identity tensor. More detailed discussion concerning these aspects of twinning can be found in (Christian & Mahajan, 1995).

According to the standard procedure twinning is described as a unidirectional slip mode, cf. Chin et al. (1969), Kalidindi (1998), Staroselsky and Anand (1998). The rate of pseudo-slip $\dot{\gamma}^{l}_{(t)}$ is calculated using the rate of volume fraction $\dot{f}^{l}$ of the twinned part created by the twin system l with the formula

$$\dot{\gamma}^{l}_{(t)} = \gamma^{\mathrm{TW}} \dot{f}^{l}. \tag{2}$$

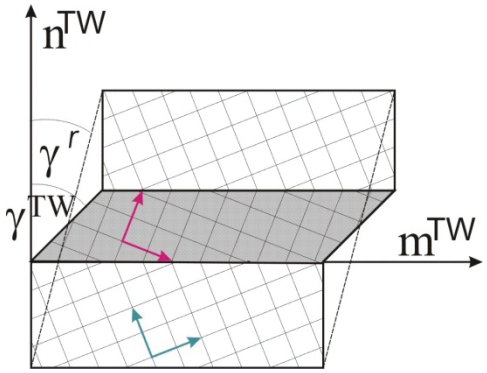

***Fig. 1**. Single grain deforming by twinning in relaxed configuration.*

The plastic part of the velocity gradient is then specified as follows:

$$\mathbf{l}^{p} = \sum_{k=1}^{2M} \dot{\gamma}^{k}_{(s)} \mathbf{m}^{k} \otimes \mathbf{n}^{k} + \sum_{l=1}^{N} \dot{\gamma}^{l}_{(t)} \mathbf{m}^{l} \otimes \mathbf{n}^{l} = \sum_{k=1}^{2M+N} \dot{\gamma}^{r}_{(s)} \mathbf{m}^{r} \otimes \mathbf{n}^{r} \tag{3}$$

where $\dot{\gamma}^{k}_{(s)}$ denotes the rate of shear in the k-th slip system. For convenient description of twin unidirectionality, the slip in **m** is distinguished from the slip in **-m** direction. The total volume fraction of twins in all twin systems should not exceed unity, i.e. $f^{\mathrm{TW}} = \sum_{l=1}^{N} f^{l} \leq 1$. Moreover, some experimental evidences for low sfe metals suggest that during the plastic straining process, first, the twin volume fraction is steadily increasing but at larger strains it reaches a saturation value considerably lower than unity, cf. Asgari et al. (1997); Kalidindi (2001); Salem et al. (2005).

2.2. Texture development

Two types of approaches developed to model texture evolution in the presence of twinning can be distinguished: a two-scale approach (Van Houtte, 1978; Tomé et al., 1991; Staroselsky and Anand, 1998; Kowalczyk-Gajewska, 2010) and a three-scale approach (Kalidindi, 1998; Proust et al., 2007; Homayonifar & Mosler, 2012). In order to emphasize the difference between the two approaches let us consider a single crystal. In the case of metals deforming only by slip, to study the texture evolution for such crystal it is sufficient to consider a single grain with an initially specified orientation. However, when metal deforms also by twinning, two significantly different families of orientations will be observed in the material: a parent one and a twin-related one.

Therefore, in order to simulate appearance of twin related orientations, according to the first approach, we initially represent our single crystal by collection of grains with the same orientation. As deformation by twinning proceeds, some of these grains assume a twin-related orientation (see figure 2a). It is well seen in figure 2 that in this way we are able to reproduce in a statistical sense the volume effect of twin related orientations on the texture image. Note also that the number of grains does not increase during the calculations, which is the main reason why researchers resort to probabilistic schemes. However, since the grain is reoriented instantaneously, the two-scale models do not account for a growth of a twin inside the grain and development of a layered substructure shown in figure 2b.

These morphological features of microstructure of metals deforming by twinning are taken into account by three-scale models. In these models three levels of microstructure are considered: an aggregate level, a single grain level within which the evolution of layered substructure is enabled, and a level of a single matrix or twin lamellae.

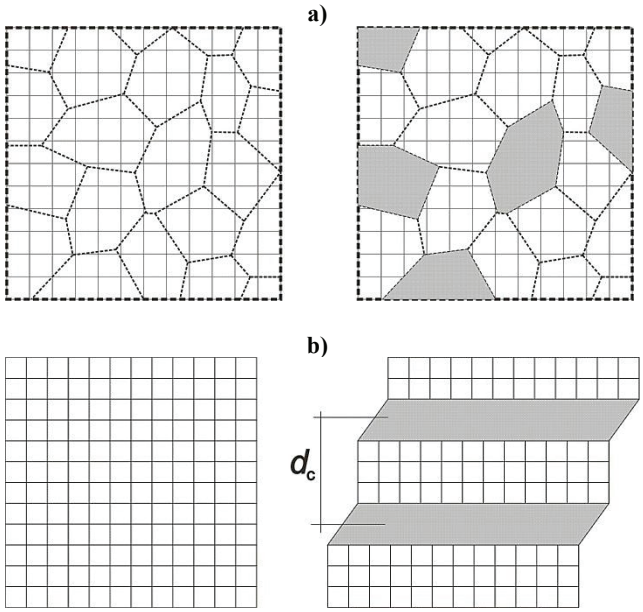

***Fig. 2.** Appearance of twin related orientations according to a) two-scale approaches b) three-scale approaches (gray domains represent the part of a volume element with a twin-related orientation).*

First let us discuss first type of approaches. Within this modelling framework a key role is played by the so-called reorientation scheme. This computational procedure specifies rules according to

which it is decided if at a given deformation step a grain stays with a matrix orientation or assumes a twin-related one. It seems to be obvious that for successful texture prediction such scheme must ensure consistency between volume fraction of grains reoriented by twinning and the accumulated volume fraction of twins f^{TW} predicted by the constitutive model.

At least five reorientation schemes can be found in the literature. They are listed below in order of appearance.

1) **The probabilistic scheme** due to Van Houtte (1978) (VH). According to this scheme, for a considered time increment, for each grain the *increment* of twin volume Δf^l on the most active twin system is compared with some number ξ. If $\Delta f^l \geq \xi$ then the corresponding grain is reoriented to take a twin-related orientation. Number ξ is randomly polled from the set $< \xi_0; 1 >$.
2) **Predominant Twin Reorientation scheme** (PTR) (Tomé et al., 1991). In this scheme the threshold value is not polled but determined from the equation

$$\xi = A_1 + A_2 \frac{F^{\mathrm{E}}}{F^{\mathrm{TW}}} \tag{4}$$

where A_1 and A_2 are two additional material constants which must be specified in experiments and denote initiation of reorientation and its saturation. In reorientation condition the value of ξ is compared with the maximum of *total* volume fractions f^l for twin systems accumulated during the whole deformation process in the considered grain. At a given deformation step the reorientation condition is checked for the subsequent grains in the aggregate as long as the volume fraction of reoriented grains F^{E} balances the *total* accumulated volume fraction of twins in the *whole* aggregate, predicted by the constitutive model, i.e. $F^{\mathrm{TW}} = \sum_{gr} f_{gr}^{\mathrm{TW}}$. This reorientation scheme is implemented in a widely used VPSC code (Lebensohn & Tomé, 1993). Note that the decision about the reorientation requires the analysis of the whole polycrystalline aggregate, therefore this scheme is not applicable to a finite element (FE) model of polycrystal.
3) **The Volume Fraction Transfer scheme** (VTR). It was also proposed in (Tomé et al., 1991). It uses a different concept of texture calculations: during the deformation the set of orientations remains fixed while only associated volume fractions evolve.
4) **The Staroselsky-Anand scheme** (SA) (Staroselsky & Anand, 1998). It follows the idea of Van Houtte but modifies it to take into account the history of a deformation process. At a given strain increment the threshold value ξ is compared with the maximum of the *total* volume fractions f^r for twin systems accumulated during the whole deformation process.
5) **The Probabilistic Twin Volume Consistent scheme** (PTVC), (Kowalczyk-Gajewska, 2010). It also follows the idea of Van Houtte and it is proposed in such a way to overcome the problem of inconsistency present in the original proposal of Van Houtte and its modification by Staroselsky and Anand. According to this proposal the interval from which the threshold value ξ is generated evolves during the process to ensure required consistency.

All these methods are formally capable of prediction of secondary and subsequent twinning events, e.g. de-twinning (Proust et al., 2009). If such events are really admitted is determined by the description of mechanical characteristics of the grain after reorientation due to twinning. It should be added that initially the number of grains in the aggregate must be larger than in the simulations of crystal plasticity without twinning in order to model the aggregate in a statistically meaningful sense.

Let us look more closely at the issue of inconsistency in the reorientation conditions originating in Van Houtte probabilistic proposal. First observe that the required consistency will be ensured when the probability of reorientation up to a given deformation step follows the total accumulated twin volume fraction predicted by the constitutive model. To verify this requirement for the three schemes of the considered type: VH, SA and PTVC, assume for simplicity single crystal deforming by twinning on the single twin system in a way that at each time step the increment of twin volume fraction is equal to Δf and that $\xi_0 = 0$ in all cases. The probability tree for reorientation problem related to this example is shown in figure 3a. Using this figure the total probability of reorientation of the grain up to time step N is specified as

$$\begin{aligned} P_N = {} & p_1 + (1 - p_1)p_2 + \ldots \\ & + (1 - p_1)(1 - p_2)\ldots(1 - p_{N-1})p_N \end{aligned} \tag{5}$$

where p_i denotes the probability of reorientation at specified time step i. For the original Van Houtte scheme p_i is equal to Δf, so that

$$P_N^{VH} = 1-(1-\Delta f)^N \neq N\Delta f = f^{\mathrm{TW}} \qquad (6)$$

while according to the Staroselsky-Anand scheme p_i is equal to $i\Delta f$, so that

$$P_N^{SA} = \left(\sum_{k=1}^{N}(k\Delta f)\prod_{j=0}^{k-1}(1-j\Delta f)\right) \neq N\Delta f = f^{\mathrm{TW}} \qquad (7)$$

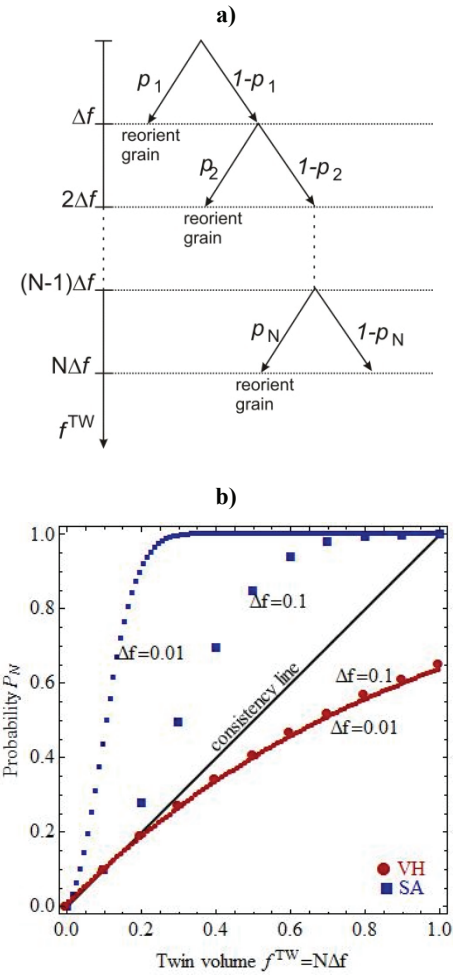

***Fig. 3**. a) Probability tree for probabilistic reorientation schemes; b) Comparison of predicted probability P_N with the accumulated twin volume fraction $f^{TW} = N\Delta f$ for subsequent time steps (VH - the Van Houtte scheme, SA - the Staroselsky and Anand concept).*

In both cases one observes inconsistency between probability of reorientation and accumulated twin volume fraction (see figure 3b). With the help of the above observation it was proposed in (Kowalczyk-Gajewska, 2010) to adjust the probability of reorientation p_i in such a way to enforce the required consistency. It was achieved by changing the interval $< 0;\Psi_i >$ from which ξ is polled in subsequent steps and compared within the total accumulated twin volume fraction at this step. The evolution of the interval is specified by employing the rule of mathematical induction: assuming that the consistency is ensured at the time step N - 1, i.e. $P_{N-1} = f_{N-1}^{\mathrm{TW}}$ and that $p_N = f_N^{\mathrm{TW}} / \Psi_N$, specify Ψ_N to ensure consistency at the time step N. As a result it is obtained that

$$\Psi_N = \frac{1-f_{N-1}^{\mathrm{TW}}}{f_N^{\mathrm{TW}} - f_{N-1}^{\mathrm{TW}}} f_N^{\mathrm{TW}} \qquad (8)$$

Reorientation condition is checked only when $\Delta f^{\mathrm{TW}} > 0$ for the considered time increment. Note that similar reasoning can be applied to ensure consistency for the Van Houtte type condition, so when the threshold value ξ is compared with a twin volume *increment* (i.e $p_N = \Delta f / \widetilde{\Psi}_N$). Then one finds

$$\widetilde{\Psi}_N = 1 - f_{N-1}^{\mathrm{TW}} \qquad (9)$$

Now, let us move to three-scale approaches developed to model texture evolution in the presence of twinning. At least three such models can be distinguished, namely:

1) **The total Langrangian approach** (Kalidindi, 1998; Salem et al., 2005) The approach uses the time-integration scheme for crystal plasticity equations in which all calculations are performed in a relaxed configuration. In this configuration the matrix grain orientation and all the twin-related orientations are predefined in terms of the initial orientation of a lattice. The same deformation gradient for the twinned and untwinned regions of the grain is assumed. As the deformation proceeds, the volume fraction of twinned regions increases. Only the matrix part of a grain can deform by slip and twinning while twinning is not possible in twinned parts. In the frame of the model, all of the twinned regions of the crystal belonging to a specified twin system would have a single lattice orientation in the current configuration, independently of the instances when they are created. The modified version of this approach employing the grain fragmentation concept was presented in (Wu et al., 2007). In the modified version initially a grain deforms as in two-scale models by slip and by twinning described as a pseudo-slip. When a certain volume fraction of twins is accumulated the grain is fragmented according to the dominant twin system. After fragmentation twinning is not al-

lowed both in the parent and the twin-related parts.

2) **The composite grain model** (Proust et al., 2007, 2009). Similarly to the modified approach of Kalidindi also within this model the layered substructure of a grain is formed according to the most active (predominant) twin system. However, the overall stress and strain rate tensors are distributed between matrix and twin lamellae according to relations valid for the laminate, cf. Stupkiewicz & Petryk (2002).
3) **The variational energy-based model** (Homayonifar & Mosler, 2012). The model follows the general concept of incremental energy minimization, cf. (Petryk, 2000), applied earlier to model for example the phase transformation phenomenon in shape memory alloys (e.g. Stupkiewicz and Petryk (2002); Bartel and Hackl (2008)) or the substructure evolution in metals deforming by multiple slip (e.g. Ortiz et al., 2000; Petryk & Kursa, 2013). Within the model the description of dislocation slip follows the classical crystal plasticity while the phase decomposition associated with twinning is accounted for by a mixture theory. The transformation of lattice orientation due to twinning (i.e. first rank lamination) takes place continuously following the energy minimization principle. The kinematic compatibility between matrix and twin phases is enforced similarly to laminate description in the composite grain model. Due to its complexity the model has not yet been applied to model texture evolution in grain aggregates composed of many grains. Only a study for single initial orientation has been performed.

The issue of matrix-twin interface is signaled at the end of this section. It is known that when twin is formed the interface between the matrix part and the twin-related part is a crystallographic plane but there are no established views if this plane remains crystallographic or behaves as a material surface (Kowalczyk-Gajewska, 2011). According to the above three-scale approaches the latter possibility is assumed.

3. CONSTITUTIVE MODELS

According to the classical Schmid law slip on the slip system is initiated when the resolved shear stress $\tau^r = |\mathbf{m}^r \cdot \boldsymbol{\sigma} \cdot \mathbf{n}^r|$ reaches the critical value τ_c^r, where $\boldsymbol{\sigma}$ is the Cauchy stress. The similar condition for twinning initiation was postulated by Chin and coworkers (Chin et al., 1969; Christian & Mahajan, 1995; Fischer et al., 2003). This hypothesis was later confirmed in experiments, for example the so-called "latent hardening experiments" performed recently on fcc single crystals by Szczerba et al. (2004). The only difference with respect to slip is that the resolved shear stress τ^l on the twin system l must satisfy the sense of the twin shear, that is, $\tau^r = \mathbf{m}^r \cdot \boldsymbol{\sigma} \cdot \mathbf{n}^r$ if $\mathbf{m}^r \cdot \boldsymbol{\sigma} \cdot \mathbf{n}^r > 0$ and is equal to zero otherwise. Below the same definition is also assumed for the resolved shear stress for a slip and, consequently, the slip in **m** direction is distinguished from the slip in **-m** direction.

Depending on the adopted formulation of crystal plasticity, the relation between the rate of slip on the slip system r or the rate of pseudo-slip on the twin system r and the resolved shear stress τ^r can take the following form (the most common formulations are invoked):

– **The classical multi-surface Schmid law** (Asaro, 1983; Van Houtte, 1978; Kalidindi, 1998; Staroselsky & Anand, 1998)

$$\dot{\gamma}^r = \dot{\lambda}^r \tag{10}$$

where $\dot{\lambda}^r$ are plastic multipliers for which complementarity and consistency conditions are satisfied:

$$\begin{aligned} &\dot{\lambda}^r \geq 0 \text{ and } f^r = \tau^r - \tau_c^r \leq 0 \text{ and} \\ &\dot{\lambda}^r f^r = 0 \text{ and } f^r \leq 0 \text{ and } \dot{\lambda}^r f^r = 0 \end{aligned} \tag{11}$$

– **The regularized Schmid law** with yield surface F of $2n$ degree (Gambin, 1992; Kowalczyk-Gajewska, 2010)

$$\dot{\gamma}^r = \dot{\lambda} \frac{1}{\tau_c^r} \left(\frac{\tau^r}{\tau_c^r} \right)^{2n-1} \tag{12}$$

where $\dot{\lambda}$ is a plastic multiplier fulfilling

$$\begin{aligned} &\dot{\lambda} \geq 0 \text{ and } F \leq 0 \text{ and } \dot{\lambda} F = 0 \text{ and} \\ &\dot{F} \leq 0 \text{ and } \dot{\lambda} \dot{F} = 0 \end{aligned} \tag{13}$$

– **Rate-dependent crystal plasticity** with a power-law relation (Asaro & Needleman, 1985; Tomé et al., 1991; Proust et al., 2007)

$$\dot{\gamma}^r = \dot{\gamma}_0 \left(\frac{\tau^r}{\tau_c^r} \right)^{\frac{1}{m}} \tag{14}$$

where m and $\dot{\gamma}_0$ are a rate sensitivity exponent and a reference slip rate, respectively.

Accumulation of dislocations makes further deformation by slip more and more difficult. In the constitutive description this fact is accounted for by the hardening rules governing the evolution of τ_c^r. The evolution of τ_c^r depends also on interactions between slip and twin systems, cf. Staroselsky and Anand (1998), Karaman et al. (2000), Kalidindi (2001). As it is observed in experiments, cf. Asgari et al. (1997), El-Danaf et al. (2001), Karaman et al. (2000), twin boundaries can be treated as grain boundaries, especially with increasing strain. Near twin boundaries pile-ups of dislocations are formed resulting in stress concentrations. This geometrical constraint on deformation leads to high latent hardening, especially for non-coplanar slip or twin systems. In most low sfe fcc materials twins cluster to form bundles a few tenths to a few micrometers thick with thin layers of matrix between them (Karaman et al., 2000). These twins do not grow to form thicker twins and they are stable after unloading. For these materials, especially in the case of high concentration of solute atoms, at larger strains the twin volume fraction appears to reach the saturation value considerably lower than unity (Asgari et al., 1997). As a result the lamellar substructure with constant thickness of matrix/twin lamellae is developed. Such fine substructure is not observed in the case of hcp materials, which twin more easily (e.g. in Mg alloy AZ31B with basal texture subjected to in-plane compression, after 10% of strain almost 90% of material has twinned and twins 'coalesce' inside the grains, cf. Proust et al. (2009)).

Modelling of hardening in the presence of twinning remains an open issue. Some contributions to the subject can be found in (Staroselsky & Anand, 1998; Karaman et al., 2000; Kalidindi, 2001; Kaschner et al., 2006, 2007; Proust et al., 2007, 2009; Wu et al., 2007; Kowalczyk-Gajewska, 2010; Capolungo et al., 2009; Beyerlein et al., 2011; Dancette et al., 2012). In general, the structure of the hardening law for materials deforming simultaneously by slip and twinning can be written in the following form

$$\dot{\tau}_c^r = \dot{\tau}_c^{r+M} = \sum_{q=1}^{M} h_{rq}^{(ss)} \dot{\bar{\gamma}}^q + \sum_{q=2M+1}^{2M+N} h_{rq}^{(st)} \dot{\gamma}^q \quad \text{for } r \le M \tag{15}$$

$$\dot{\tau}_c^r = \sum_{q=1}^{M} h_{rq}^{(ts)} \dot{\bar{\gamma}}^q + \sum_{q=2M+1}^{2M+N} h_{rq}^{(tt)} \dot{\gamma}^q \quad \text{for } r > 2M, \quad \dot{\bar{\gamma}}^q = \dot{\gamma}^q + \dot{\gamma}^{q+M} \tag{16}$$

and the self and latent hardening submatrices $h_{rq}^{(\alpha\beta)}$ account for the interactions of the deformation mechanisms of the slip-slip *(ss)*, slip-twin *(st)*, twin-slip *(ts)* and twin-twin *(tt)* types. In order to account for the discussed difference between the hardening due to slip or twinning on co-planar and non-coplanar slip/twin systems usually the following form of these submatrices is assumed (Asaro & Needleman, 1985; Anand, 2004; Kalidindi, 2001; Kowalczyk-Gajewska, 2010),

$$h_{rq}^{(\alpha\beta)} = H_{(\alpha\beta)}^r \left(q^{(\alpha\beta)} + \left(1 - q^{(\alpha\beta)}\right) \left| \mathbf{n}^r \cdot \mathbf{n}^q \right| \right) \tag{17}$$

where $q^{(\alpha\beta)}$ are the latent hardening ratios which could be different depending on the type of interactions *(αβ)*. The coefficient $H_{(\alpha\beta)}^r$ is the current hardening modulus of the *r*-th slip or twin system due to activity of other slip or twin systems.

The formula most often used for describing the current hardening modulus $H_{(ss)}^r$ due to slip-slip interaction is the the Voce-type law with saturation (Kalidindi et al., 1992), namely,

$$H_{(ss)}^r = h_0^{ss} \left(1 - \frac{\tau_c^r}{\tau_{sat}^r} \right)^{\beta} \tag{18}$$

The relation describes the athermal statistical storage of moving dislocations and dynamic recovery. For $\beta = 1$ the exponential hardening rule is obtained. Quantities h_0^{ss}, τ_{sat}^r, β are material parameters.

Staroselsky and Anand (1998) used a similar law to describe the remaining modulae assuming different values for parameters h_0, τ_{sat} and β. In their work slip-twin and twin-twin interactions are enabled after some volume fraction of twins is accumulated.

In (Kalidindi, 2001; Salem et al., 2005) slip-twin interactions are not described directly but the parameters h_0^{ss}, τ_{sat}^r and β in (18) depend on the accumulated twin volume. The power law is used to describe the current modulae $H_{(t\beta)}^r$ namely

$$H^r_{(t\beta)} = h^0_{t\beta}\left(\hat{\dot{\gamma}}^{\beta}\right)^{n\beta}, \text{ where}$$
$$\hat{\dot{\gamma}}^{\beta} = \begin{cases} \sum_{r=1}^{M}\left|\dot{\gamma}^t\right| & \text{for } \beta = s \\ \sum_{r=l}^{N}\gamma^{\mathrm{TW}}\dot{f}^l & \text{for } \beta = t \end{cases} \quad (19)$$

A physically-based hardening model for twin-twin and slip-twin interactions was proposed in (Karaman et al., 2000). The geometrical effect of twin boundaries on hardening is accounted for by a term which is proportional to $f^{\mathrm{TW}} / (1- f^{\mathrm{TW}})$. The corresponding proportionality factor is specified by the constant K_0 and the inverse of the average thickness of twin lamellae t - the first length scale parameter. For polycrystalline materials, an additional term is introduced depending on the second length scale parameter - the grain size.

Following the above formulation, in Kowalczyk-Gajewska (2010, 2011) the current modulae $H^r_{(\beta t)}$ have been specified as

$$H^r_{(\beta t)} = \frac{h_0^{\beta t}}{\tau_c^r}\left(\frac{f^{\mathrm{TW}}}{f_{sat}^{\beta t} - f^{\mathrm{TW}}}\right) \quad (20)$$

where $h_0^{\beta t}$ and $f_{sat}^{\beta t} \le 1$ are material parameters. The hardening of twin systems due to slip activity is neglected or accounted for by a simplified linear law ($H^r_{(ts)}$ = const). Schematically, the evolution of τ_c due to slip activity and twin activity in this approach is presented in figure 4. It must be noted that the variation of τ_c with increasing twin volume fraction is the same as those obtained using (Karaman et al., 2000) formulation.

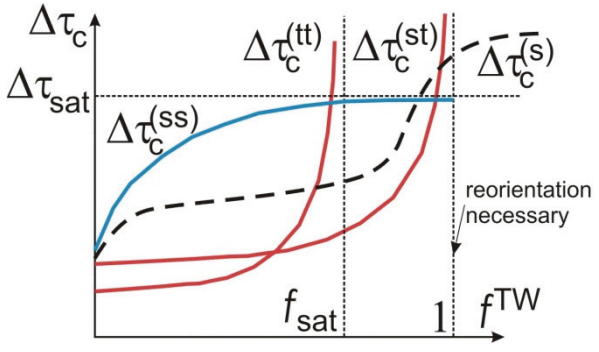

Fig. 4. *Schematic view of evolution of critical shear stress τ_c due to slip activity and due to twin activity ($f_{sat}^{st} = 1$) postulated in (Kowalczyk-Gajewska, 2010). The dashed line shows resulting total evolution of the critical shear stress for slip (when $f^{TW} = 1$ the grain is inevitably reoriented, so the level of $\Delta\tau_c$ for $f^{TW} > 1$ represents assumed mechanical characteristics of a grain after reorientation).*

The use of a two-scale model with the reorientation condition requires one also to specify if slip and twinning may take place in the grains reoriented by twinning, and what are slip and twin resistances after reorientation. As concerns low sfe materials experimental observations by Asgari et al. (1997) and Karaman et al. (2000) indicate that twinning and slip within the twinned regions are at least more difficult than in the untwinned part and, moreover, slip in the twinned regions can be severely restricted to the planes that are coplanar with the matrix-twin boundary. It is explained by the Hall-Petch type effects induced by the directional reduction of the mean free path (mfp) in a twin platelet, cf. Mahajan and Chin (1973). Alternative explanation is provided by Basinski's mechanism (Basinski et al., 1997): twinned regions are harder because the glissile dislocations before twinning are converted into sessile dislocations due to the twinning shear transformation. Both mechanisms were evaluated by Salem et al. (2006) for high purity titanium (hcp material). Microhardness tests showed that twins were significantly harder than matrix, while nanoidentation measurements indicated no clear correlation between the hardness of twins and slip distance/twin thickness. These observations were in favour of Basinski's mechanism. In order to account for the above-mentioned phenomena in the twinning modelling the mechanical characteristics of grains after reorientation are usually modified with respect to the ones of a matrix grain. For example, Staroselsky and Anand (1998) assume that after the reorientation the values of τ_c^r for all twin systems are equal to the value of τ_c for the twin system, according to which the reorientation takes place, while the values of τ_c^r for all slip systems are equal to the value of τ_c for the slip system coplanar with the reorientation twin system. Twinning is thus admissible in the reoriented grains, which corresponds to the possibility of twinning in the twinned part of the grain. Contrary, Kalidindi (1998, 2001) does not enable twinning in the reoriented grain, while Karaman et al. (2000) increase all slip and twin resistances by 20% in the reoriented grains.

In (Proust et al., 2007) the hardening description makes use of a 3-scale model of polycrystal deforming by twinning. The evolution of critical shear stress is composed of three terms: the evolution of statistical dislocations (STAT) governed by formula (18), the evolution of geometrically necessary dislocations (GND) and a directional Hall-Petch effect

(HP). The second and third terms are affected by slip-twin interactions. The evolution of a GND term follows the work of Karaman et al. (2000), i.e.

$$\dot{\tau}^r_{GND} = \frac{h^r_m}{d^r_{mfp}\left(\tau^r_{STAT} + \tau^r_{GND}\right)}\dot{\gamma}^r \qquad (21)$$

where d^r_{mfp} is a mean free path calculated considering a layered substructure of a composite grain, namely (see figure 2)

$$d^l_{mfp} = f^{\mathrm{TW}}_{\max} d_c / \sin\alpha, \quad d^k_{mfp} = \left(1 - f^{\mathrm{TW}}_{\max}\right) d_c / \sin\alpha \qquad (22)$$

for twin and slip systems, correspondingly ($f^{\mathrm{TW}}_{\max}$ - the twin volume for predominant twin system, α - the angle between the matrix-twin interface and the slip or twin plane of the system *k* or *l*). This quantity is also used in the HP term of the familiar form

$$\tau^r_{HP} = \frac{h^r_{HP}}{\sqrt{d^r_{mfp}}} \qquad (23)$$

h^r_m and h^r_{HP} are material parameters. Initially, it was proposed to use the same relations for slip and twin systems, however, in (Proust et al., 2009) a simple exponential hardening was used for twinning systems. A directional mean free path was also a decisive parameter in the hardening description proposed for TWIP steels in (Dancette et al., 2012).

In (Capolungo et al., 2009) the composite grain model was applied to zirconium. It was noticed that twin propagation is preceded by twin nucleation. In the model used the transition between the two mechanisms can be described only phenomenologically. The following relation was proposed for the critical shear stress for twin systems

$$\tau^l_c = \tau^l_{nucl} + \left(\tau^l_{prop} - \tau^l_{nucl}\right) P_{nucl} + \tau^l_{slip} \qquad (24)$$

where P_{nucl} is probability that local stress is high enough to activate twinning nucleation. For $P_{\mathrm{nucl}} = 1$ regime is switched to twin propagation with a critical shear stress $\tau^l_{prop} < \tau^l_{nucl}$; τ^l_{slip} reflects twin-slip interactions. A more refined model of twin nucleation from grain boundaries and propagation was presented in (Beyerlein et al., 2011) and incorporated into the visco-plastic self-consistent (VPSC) modelling scheme. The proposal is formulated on the physically-based idea that twins originate from a statistical distribution of defects in the grain boundaries.

This modelling framework goes in line with experimental observations concerning twinned material, reported by Wang and Huang (2007) and Proust et al. (2009) for magnesium. This material shows a high propensity to twinning and the grain can be even totally transformed by its activity. Upon a strain-path change twinned grains can detwin easily. Experimental data reported by Lou et al. (2007) suggest that detwinning is easier to initiate than twinning as far as the matrix/twin interface already exists within the material, so its nucleation is not necessary. As concerns twin-slip interactions in hcp materials, it was also observed for magnesium that prior deformation by slip does not prevent deformation by twinning when the strain path is changed, although the stress level at which twinning is activated can be increased by the presence of dislocations.

At the end of this section let us shortly discuss the micro-macro transition scheme used to obtain macroscopic response of a polycrystalline material, i.e. a scale transition rule between the level of a single grain in 2-scale models, or a composite grain with layered substructure in 3-scale models, and a macroscopic level of polycrystal. The most common Taylor model, assuming the same deformation in each grain, usually does not provide acceptable results in the case of materials under consideration. Metals deforming by slip and twinning often have less than five independent easy slip systems, which leads to an overestimation of the overall stress when using the Taylor model. The self-consistent schemes, e.g. VPSC, making use of the Eshelby solution (1957), provide better estimates. Note that for non-linear material behaviour different variants of the self-consistent approach are available. They are not discussed here in more detail. The reader is referred to the related publications, e.g. (Molinari et al., 1997; Masson et al., 2000; Kowalczyk-Gajewska, 2011). The multi-site ALAMEL model accounting for short-range interactions between neighboring grains can also be used (Van Houtte et al., 2005; Dancette et al., 2012).

4. EXAMPLE

Below an example of -TiAl intermetallic is used to illustrate the capabilities of the crystal plasticity approach in predicting the properties of a material deforming by slip and twinning. We use here the results presented in (Kowalczyk-Gajewska, 2011), discussed there in slightly different aspects. We start

with the theoretical analysis enabling the prediction of deformation modes to be active during the performed processes, e.g. experimental tests. In our opinion such a theoretical analysis should precede the establishment of an efficient testing strategy.

As can be observed in table 1 three types of deformation modes are possible for γ -TiAl intermetallic. Let us introduce notation: $\alpha^{ord} \equiv \tau_c^{ord} / \tau_c^{\sup}$ and $\alpha^{tw} \equiv \tau_c^{tw} / \tau_c^{\sup}$, where $\tau_c^{ord}, \tau_c^{\sup}$ and τ_c^{tw} are critical shear stresses for ordinary, superdislocations and twinning, respectively. The slip systems belonging to the superdislocation category are sufficient to perform any isochoric shape change of the volume element of the single crystal. On the other hand, some deformation paths are not possible using only ordinary dislocations and twinning systems. For some combinations of ratios α^{ord} and α^{tw}, twinning and ordinary dislocations will never be activated. To show that, let us assume a shear stress specified by one of the slip systems belonging to one of two considered categories, i.e. $\boldsymbol{\sigma} = \tau^K / 2\left(\mathbf{m}^k \otimes \mathbf{n}^k + \mathbf{n}^k \otimes \mathbf{m}^k\right)$, and calculate the yield stress τ_Y^K of single crystal for such stress state. For shear specified by one of ordinary dislocations and for one of the twin systems, it is respectively obtained:

$$\frac{\tau_Y^I}{\tau_c^{\sup}} = \min\left\{\alpha^{ord}, 2, 3\sqrt{3}\alpha^{tw}\right\},$$
$$\frac{\tau_Y^{II}}{\tau_c^{\sup}} = \min\left\{3\sqrt{3}\alpha^{ord}, \frac{2}{\sqrt{3}}, \alpha^{tw}\right\} \qquad (25)$$

so that ordinary dislocations are not initiated if $\alpha^{ord} > 2$, while twinning is not initiated if $\alpha^{tw} > 2/\sqrt{3}$. A more detailed analysis concerning modes activity in γ - TiAl as well as its influence on the yield surface can be found in Mecking et al. (1996). However, at room temperature, most of experiments indicate that $\alpha^{ord} < \alpha^{tw} < 1$, cf. Appel and Wagner (1998), so that ordinary dislocations and twinning are easy deformation modes. The observed low formability of the material is thus caused by the fact that the number of independent easy slip systems is lower than five.

The properties of commercially processed γ -TiAl alloy were investigated within KMM NoE project (www.kmm-noe.org). Using scanning electron microscopy (SEM) and neutron diffraction measurements it was verified that the material had near gamma equiaxed microstructure without texture (KMM NoE, 2007b). Then tension and compression tests were performed at room temperature using different strain-rates (KMM NoE, 2007a). It was found that the strain-rate sensitivity was not significant for the moderate strain-rates (0.4-0.004[1/s]). Limit strains in tension did not exceed 3%, while in compression tests strain up to 35% was achieved. Unfortunately, the final texture after compression was not measured. Therefore the identification of material parameters was supported by the results concerning the texture after compression up to 30% reported by Wang et al. (1997) (see figure 8a) for similar material.

The experimental compression texture of γ -TiAl shows asymmetry between the components <*h*0*k*] and <*hk*0]. It is not observed for fcc materials for which equal concentrations of poles around all <110> directions is found. The inverse pole figure presented in figure 8a contains two important components: the first one is 10° away from <101] directions with a spread of 5° in the pole figure; the second one is a strong <*hk*0] fibre texture running from <010] to <100] directions. The poles belonging to this fibre show tendency to concentrate around <110] direction (more details can be found in (Wang et al., 1997)). Asymmetry of texture can be linked with a different status of ordinary dislocations and superdislocations. Moreover, as discussed by Bartels et al. (2002), shifting of the first maximum from <101] to another orientation <302], as well as the appearance of orientations around <100] can be explained by the twinning activity. Below we will show that by consistent crystal plasticity modelling we are able to support these hypotheses.

***Table 2**. Identified material parameters for γ -TiAl of near gamma microstructure (material tested within KMM NoE project (KMM NoE, 2007a)). Identification performed for the Taylor/VPSC model of polycrystal (if single value is placed in the table, it means that the same value of the parameter was used for both models), τ_{c0}^{ord} = 77.5 MPa / 142 MPa, n = 20 in Eq. (14).*

Mode	Interactions	$\tau_{c0}\left[\tau_{c0}^{ord}\right]$	$h_0\left[\tau_{c0}^{ord}\right]$	$\tau_{sat}\left[\tau_{c0}^{ord}\right] / f_{sat}$	a	q
Ord.	slip-slip	1.0	6.0/5.0	25./20.	1.1	1.0
	slip-twin	—	1.0	1.0	—	1.6
Super.	slip-slip	5.0/2.0	6.0/5.0	500./45.	1.1	1.0
	slip-twin	—	1.0	1.0	—	1.6
Twin	twin-slip	—	0.	—	—	0.0
	twin-twin	1.25/1.1	6.0/4.0	0.4/0.5	—	1.6

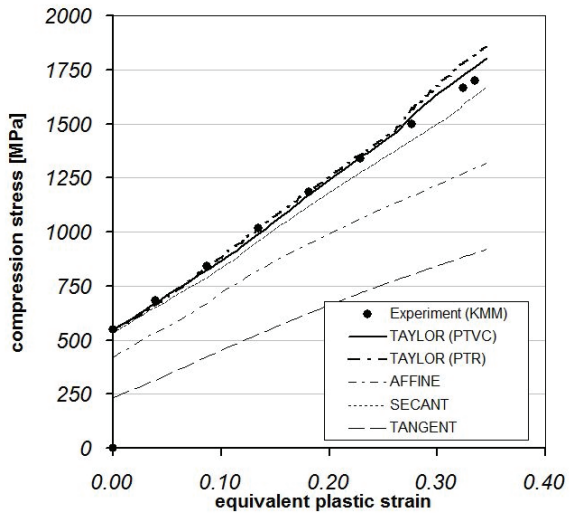

***Fig. 5**. Simple compression: axial stress vs. equivalent plastic strain curves, material parameters from table 2 for Taylor model.*

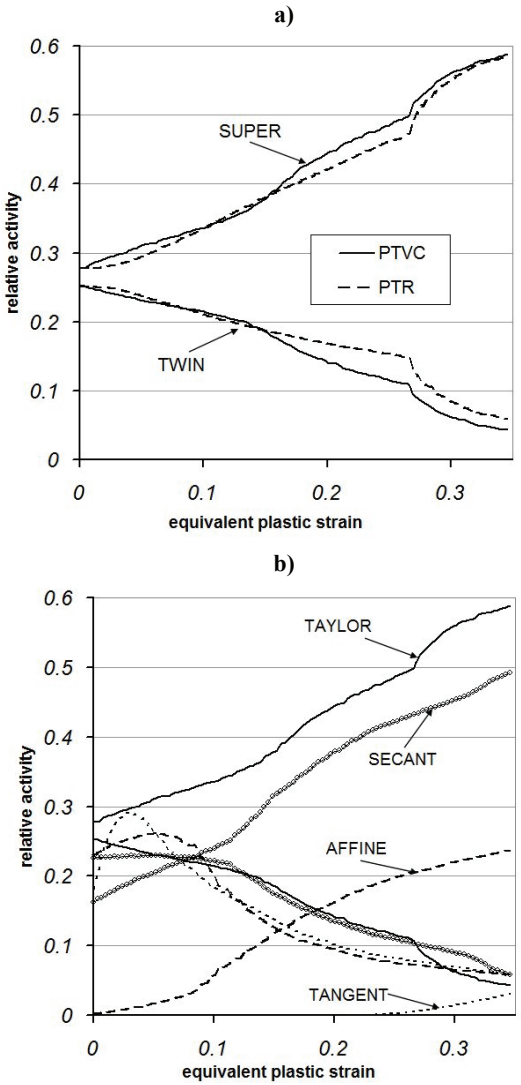

***Fig. 6**. Current relative activities of twinning and superdislocation modes: (a) comparison of PTVC and PTR schemes for Taylor model; (b) comparison of different scale transition rules (PTVC scheme, curves with annotations are for superdislocations), material parameters from table 2 for Taylor model.*

The main goal of the present study is to illustrate the strong impact of the relative activities of three categories of deformation modes and their evolution on the final texture image, as well as to indicate the important factors influencing the results in view of the applied modelling framework (e.g. a reorientation scheme, a hardening rule, an averaging scheme). It must be stressed that because the available experimental results are by far insufficient, quantitative predictions of the presented modelling must be taken with care.

Two sets of material parameters have been identified on the basis of the compression test for the lowest strain rate: the first one under the assumption of the Taylor model of polycrystal and the second one under the assumption of the VPSC model. In both cases it is assumed that material has initially no texture (random distribution of orientations in the aggregate is assumed). The parameters are collected in table 2. The simulated stress-strain responses are compared to the experimental curves in figure 5 and 9, while the final texture in figure 8. The influence of the averaging scheme can be analyzed with help of figure 5 in which with use of the same material parameters (identified for the Taylor model) calculations are performed for three different variants of the VPSC model: tangent, affine and secant. The stress level predicted by the secant variant is close to the Taylor model, the stress level predicted by the tangent variant is the lowest, while the affine variant predicts the stress level between the predictions of secant and tangent variants. This result is in agreement with available theoretical analyses, cf. Masson et al. (2000). The apparent difference between all four predictions is understood when we look at the predicted relative activity of easy and hard deformation modes presented in figure 6b. As concerns the Taylor model, high activity of hard superdislocation mode is predicted even though $\tau_c^{\sup} / \tau_c^{ord} = 5$. This activity increases in the course of deformation with decreasing activity of twinning caused by limited ability of the latter mode to carry the deformation. The activity of superdislocations in the case of the secant VPSC model is comparable with that predicted by the Taylor model, while the activity of superdislocations is almost not observed for the tangent VPSC model. The twinning activity for all four micro-macro transition schemes is comparable.

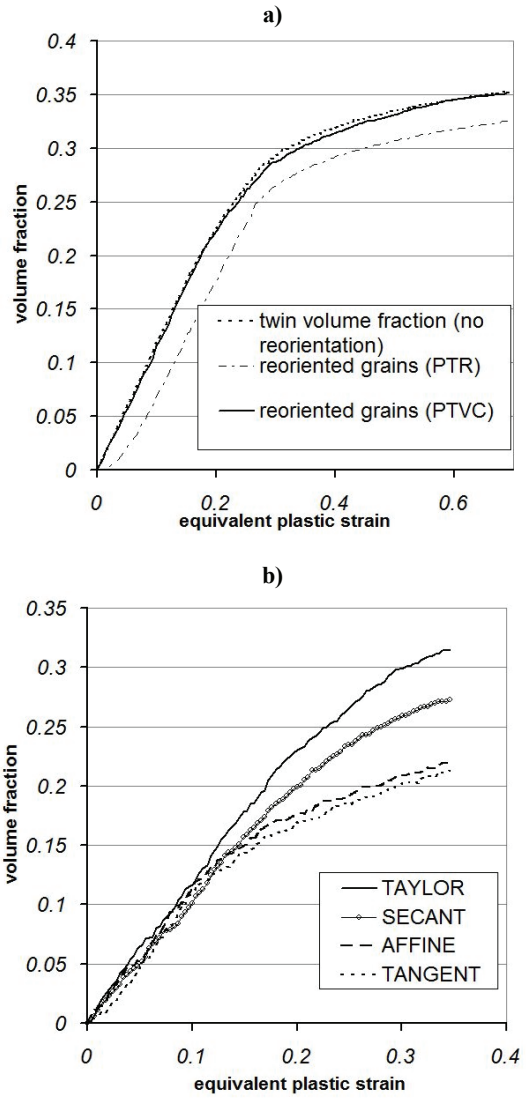

Fig. 7. *Volume fraction of reoriented grains in compression: a) Comparison of PTVC and PTR schemes for Taylor model; b) comparison of different scale transition rules (PTVC), material parameters from table 2 for Taylor model.*

The differences in activities have a direct impact on the obtained textures (figure 8). The Taylor model is able to reproduce the presence of <*hk*0] fibre, however, the texture component <302] is not predicted. Instead, the concentration of poles between <001] and <101] directions is observed. This deficiency of predictions can probably be attributed to the general inability of the Taylor model to reproduce some details of texture, cf. Kocks et al. (2000). As a solution the VPSC model is often indicated. The results obtained for different variants of VPSC are presented in figure 8d-f (material parameters as for the Taylor model). One can see that the <*hk*0] fibre component in the texture is connected with the activity of superdislocations (it almost disappears for the tangent model for which the activity of this mode is the smallest), while the changes in activity of twinning moves <101] component towards <302] component. A valid prediction of the location of this component is observed only for the affine and tangent VPSC models.

It is seen that the correct assessment of the twin volume fraction can be decisive for valid texture predictions. In figure 7b the evolution of twin volume fraction is presented (i.e. the fraction of reoriented grains in the aggregate) for all models. It is the highest for the Taylor model and the lowest for the affine and tangent models. The calculations were performed using the PTVC reorientation scheme.

The above observations indicate that the VPSC model should provide better results concerning texture evolution. This is a common conclusion for the materials of high specific strength with insufficient number of independent slip systems. The VPSC model enables strain heterogeneity within the aggregate. Therefore, the identification procedure has been performed for the affine variant of VPSC model which provided the best results in the preliminary analysis (see table 2). The critical shear stress for superdislocations is set only two times higher than that for ordinary dislocations in order to reproduce the <*hk*0] fibre component in the compression texture. Moreover, the critical shear stress for twinning is only 10% higher than τ_c^{ord}, and the value of f_{sat} is increased to 0.5 in the self-hardening function for the twinning mode. An increase of propensity to twinning has been obtained as a result. The simulated stress-strain curve, twin volume fraction and relative activities are presented in figure 9, while the final texture in figure 8g,h. Good agreement concerning the two main components of texture reported by Wang et al. (1997) is observed.

At the end let us show the difference in the results obtained with use of two reorientation schemes: the widely used PTR scheme (Tomé et al., 1991) and the PTVC scheme proposed in (Kowalczyk-Gajewska (2010)). The PTR scheme requires the specification of two additional material constants describing the accumulated twin volume fractions at which the twin-induced reorientation of grains starts and ends. In agreement with the material parameters present in a self-hardening rule for twinning (see table 2), these parameters are assumed as $A_1 = 0$ and $A_2 = 0.35$ (for Taylor identification) or $A_2 = 0.5$ (for VPSC identification). It is observed in figure 7b that in the case of PTR scheme the fraction of reoriented grains follows roughly the evolution of twin volume fraction, however, the agreement between the two is less satisfactory than in the case of the PTVC scheme. It has its impact on the relative activity of

the deformation modes presented in figures 6a and 9b as well as on the texture image for which a comparison is shown in figure 8.

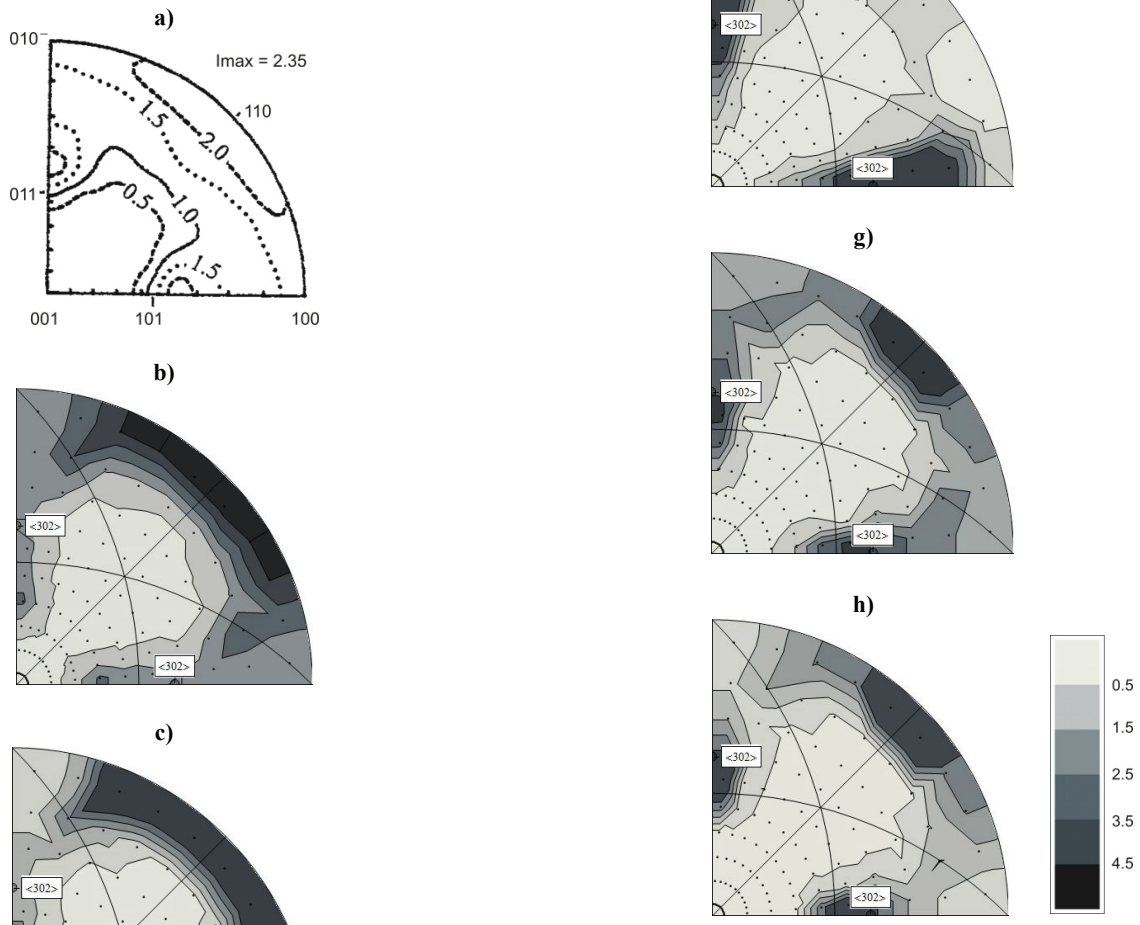

***Fig. 8**. Simple compression of TiAl, $\varepsilon = 0.3$. Inverse Pole figure (001), stereographic projection: (a) Experiment (details see (Wang et al., 1997)) (b) Taylor model - PTVC scheme, (c) Taylor model - PTR scheme, (d) Secant, (e) Affine, (f) Tangent VPSC models with PTVC scheme, material parameters for Taylor model (table 2); (g) Affine VPSC model – PTVC scheme, (h) Affine VPSC model - PTR scheme; material parameters for affine VPSC model (table 2). Contours at multiplicities of random distribution indicated by the legend.*

5. SUMMARY

The review of different modelling tools developed to account for twinning in crystal plasticity models has been presented. Two-scale and three-scale approaches proposed to model texture evolution in the presence of twinning have been discussed. The issue of consistency between accumulated twin volume fraction and volume fraction of twin-related orientations in the aggregate has been addressed. The description of coupling between two different mechanisms of plastic deformation, dislocations and twinning, has been also analyzed for different hardening law formulations available in the literature. Some of the modelling tools have been illustrated on the example of titanium aluminide.

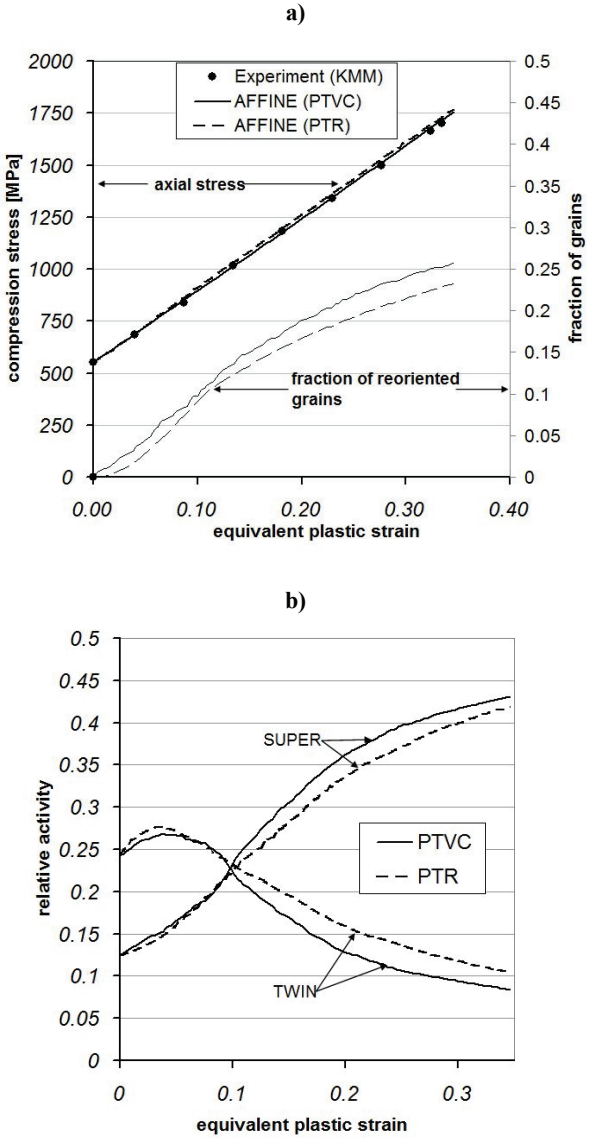

***Fig. 9**. (a) Stress-strain curves and evolution of fraction of reoriented grains; (b) Current relative activities of super-dislocations and twinning. Simple compression, affine model, PTVC and PTR schemes, material parameters from table 2 for VPSC affine model.*

As already stressed, the modelling of deformation twinning remains an open issue. The research effort is now concentrated on the three-scale models that directly account for layered substructure of grains deforming by twinning (Salem et al., 2006; Proust et al., 2009; Homayonifar & Mosler, 2012). In this respect an energy minimization approach developed recently by Homayonifar and Mosler (2012) seems to be promising, although the problem of computational efficiency must be solved for this model. On the other hand, as the most computationally efficient tools for modelling of texture, that still provide reasonable results, two-scale models can be recommended that ensure twin volume consistency, that is the PTR and PTVC schemes. Due to their statistical nature they should be used only when the assessment of the volume effect of twinning on the texture image is sufficient while the spatial distribution of matrix and twin orientations is of negligible importance.

In relation to hardening description, physically-based models of coupling between slip and twinning that differentiate between the twin nucleation and propagation as well as between the influence of twinning on statistically stored and geometrically necessary dislocations density e.g. Capolungo et al. (2009), Beyerlein et al. (2011), Dancette et al. (2012) are supposed to be the most accurate at this moment. It should be noted that a refined hardening description that implicitly takes into account the directional effect of the created layered substructure, improves the predictions of two-scale models, not only as concerns the overall stress-strain response but also the texture evolution (Kowalczyk-Gajewska, 2010). Finally, the important role of micro-macro transition scheme applied between the grain level and polycrystal level should be stressed. For materials deforming by slip and twinning the Taylor model should be avoided, while the self-consistent scheme or other scheme enabling the strain heterogeneity when going from grain to grain should be used instead.

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MODELE PLASTYCZNOŚCI KRYSZTAŁÓW UWZGLĘDNIAJĄCE MECHANIZM BLIŹNIAKOWANIA

Streszczenie

W pracy przedyskutowano istniejące metody pozwalające na uwzględnienie bliźniakowania w ramach modelu plastyczności kryształów. W szczególności przeanalizowano trzy zasadnicze problemy wymagające rozwiązania w przypadku modelowania metali i stopów, w których mamy do czynienia z tym mechanizmem deformacji plastycznej: modelowanie rozwoju tektury krystalograficznej, wpływ sprzężeń zachodzących pomiędzy mechanizmami poślizgu i bliźniakowania na sformułowanie prawa umocnienia oraz wpływ tworzącej się substruktury lamelarnej (płytkowej) na makroskopową odpowiedź materiału. Niektóre z omawianych podejść zostały zilustrowane na przykładzie związku międzymetalicznego Ti-Al.

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