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MATERIAL CRYSTAL PLASTICITY AND DEFORMATION TWINNING

Abstract. In classical crystal plasticity, the lattice orientation is unchanged from the reference configuration to the local to the local intermediate is plastically deformed configuration. Material plasticity corresponds to a different irreversible process by which the lattice rotates together with material lines between reference and intermediate configurations. Deformation twinning is an example of material plasticity. A continuum model for mechanical twinning of single crystals is presented in this work. Twin formation is regarded as an unstable localization phenomenon, followed by twin front propagation. Finite element simulations are provided showing the twinning and untwinning of a single crystal under cyclic loading, the development of twins at a crack tip, and lastly the formation of twin networks in a coating on an elastic substrate.

1. Material vs. dislocation-based crystal plasticity

The constitutive framework of anisotropic elastoplasticity has been settled by Mandel in [11]: it requires the definition of a tryad of directors attached to each material point. In the case of single crystal plasticity, the relative rotation rate of lattice directors with respect to material lines is derived in a unique way from the kinematics of plastic glide according to N slip systems. A unique intermediate configuration can be defined for which the lattice orientation is the same as the initial one. This results in a multiplicative decomposition of the deformation gradient $\underset{\sim}{\mathbf{F}}$ into elastic and plastic parts, as shown on figure 1a:

$$\underset{\sim}{\mathbf{F}} = \underset{\sim}{\mathbf{E}}\,\underset{\sim}{\mathbf{P}}, \qquad \dot{\underset{\sim}{\mathbf{P}}}\,\underset{\sim}{\mathbf{P}}^{-1} = \sum_{s=1}^{N} \dot{\gamma}^s \underline{\mathbf{m}}^s \otimes \underline{\mathbf{n}}^s$$

where slip system s is described by the slip direction $\underline{\mathbf{m}}^s$ and the normal to the slip plane $\underline{\mathbf{n}}^s$, and γ^s denotes the amount of associated slip. It follows that from the reference configuration to the intermediate one, the lattice directions are left unchanged whereas the material lines rotate according to the rotation part in the polar decomposition of $\underset{\sim}{\mathbf{P}}$.

One can also imagine an irreversible deformation process by which the lattice directions of the crystal would simply follow the material lines. This is what we call *material crystal plasticity*. It leads to the picture of figure 1b where the individual atoms undergo a uniform simple glide in a cooperative way. However this process is not so simple as it may look since during the shearing the lattice structure is changed usually going from a highly symmetric class to a less symmetric one. Some critical shear amount γ_0 may exist for which the crystal structure is retrieved with possibly an orientation different from the initial one ([14]). Such a deformation process exists

*The authors want to thank Prof. André Pineau for many discussions on twinning phenomena in zinc.

in some crystals. It is referred to as *deformation twinning* ([2, 16]). The sequel of the paper is devoted to the continuum modelling of this particular mode material crystal plasticity.

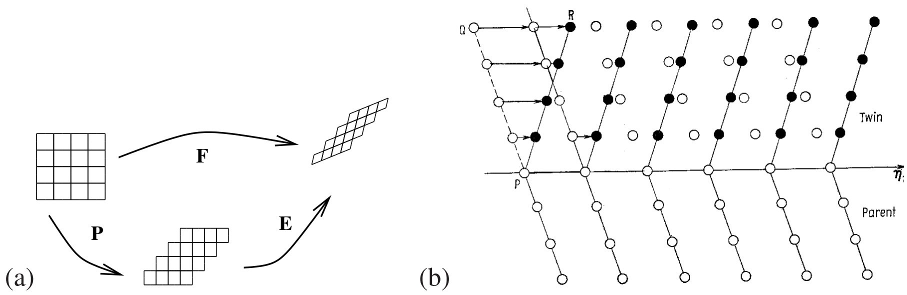

Figure 1: Kinematics of crystal plasticity based on dislocation glide (a); homogeneous shearing of a lattice as an example of material crystal plasticity (b).

Figure 2: Twin network and four cleavage cracks in a large flat zinc grain coated on a steel sheet (grain size : 500μm).

2. Continuum modelling of deformation twinning

2.1. Elements of deformation twinning

Deformation twinning now is a well–known deformation mechanism in cubic and hexagonal crystals. A modern and exhaustive account of the current knowledge from the crystallographic, metallurgical and mechanical point of view can be found in [3]. We will simply retain the following features:

• the deformation of the twinned part of the crystal can be described by a homogeneous shearing γ_0 in direction η_1 and in the plane S;

• the crystal structure of the twin usually is the mirror image of the parent crystal in the crystallographic twin plane K_1; K_1 very often coincides with the plane of contact between the two crystals called composition plane which is neither rotated nor distorted; the direction in S undergoing only a rotation is called η_2 and K_2 denotes the plane containing η_2 and normal to S;

• in fact, a simple shear applied to atom positions, as distinct from lattice points, is not always capable of producing all the atom movements which are needed to form a twin: additional *reshuffle* of some atoms of the unit cell is necessary, in particular in multiple lattices.

For simplicity, the present work is actually restricted to compound twins for which all elements K_i, η_i are rational ([10]). More specifically, the provided examples deal with pure zinc having hexagonal closed–packed symmetry. Using classical index notations for this type of symmetry ([2]), the twinning system of pure zinc is given by:

$$\eta_1 =< 10\overline{1}\overline{1} >,\ K_1 = \{10\overline{1}2\},\ \eta_2 =< \overline{1}01\overline{1} >,\ K_2 = \{\overline{1}012\},\ \gamma_0 = 0.139$$

The lattice orientation relationship between the parent crystal and the twin in zinc are: a mirror symmetry in K_1, or equivalently a rotation of angle π around η_1, a mirror symmetry in the plane normal to η_1 or a rotation of angle π around the normal to K_1.

2.2. Elastoplastic model of twinning

Mechanical models for twinning are available from both microscopic and macroscopic points of view. At the level of the cooperative behaviour of atoms, non–linear elasticity with a non–convex potential has proved to be an efficient method to describe such a phase transition–like process ([4, 19]). Indeed *elastic twinning* exists if there are no lattice friction forces opposing the motion of the dislocations at irregular interfaces. In this case, twins will run back when the applied stress is removed. In calcite for instance, small twins nucleate by indentation and disappear when the load is removed ([10]). However, more generally twinning is *not reversible* and twins remain in a crystal after it has been unloaded. The reason often is that accommodation has occurred by slip, relieving the stresses at the edge of the twin. Under these conditions, blunt twin plates with quite irregular interfaces are possible (figure 2). That is why deformation twinning is modelled here as an elastoplastic process associated with dissipation. Such an approach has already been proposed to model at the macroscopic level the volume fraction of twins appearing in a polycrystalline volume element of metal deforming by both slip and twinning ([9, 18]). We tackle here a different problem since the aim is to simulate the nucleation and propagation of twins at the grain level.

The classical framework of crystal plasticity is now extended to incorporate the following features of twinning (figure 3):

• twin formation is modelled as an unstable plastic slip process according to classical dislocation–based crystal plasticity;

• as soon as a critical amount of shear $\gamma = \gamma_0$ has been reached for the activated twin system, the orientation of the isoclinic intermediate configuration is changed switching from the initial parent one to that of the associated twin.

The driving force for twinning is the resolved shear stress τ on the twin plane in the twinning direction and the slip rate is computed using:

$$\dot{\gamma} = < \frac{\tau - \tau_c}{K} >^n, \quad \tau_c = \tau_0 + Q(1 - e^{-b(\gamma - E(\gamma/\gamma_0))})$$

where the viscosity parameters K and n are chosen so that the resulting behaviour is as rate–independent as necessary. τ_0 denotes the initial threshold for twinning and the hardening parameter Q is taken negative. Such a softening behaviour makes twin nucleation an unstable deformation mode associated with strain localization. The function floor $E(.)$ taking the integer part of . is introduced so that the initial threshold is recovered once the local twinning process is finished. Contrary to the classical Schmid law in dislocation - based plasticity, the sign of τ plays a role since twinning is possible only in one specific direction : compression in direction $\underline{\mathbf{c}}$ in zinc triggers deformation twinning, but not tension. The choice of $\underline{\mathbf{m}}$ and $\underline{\mathbf{n}}$ is such that τ, γ and $\dot{\gamma}$ are positive when twinning occurs.

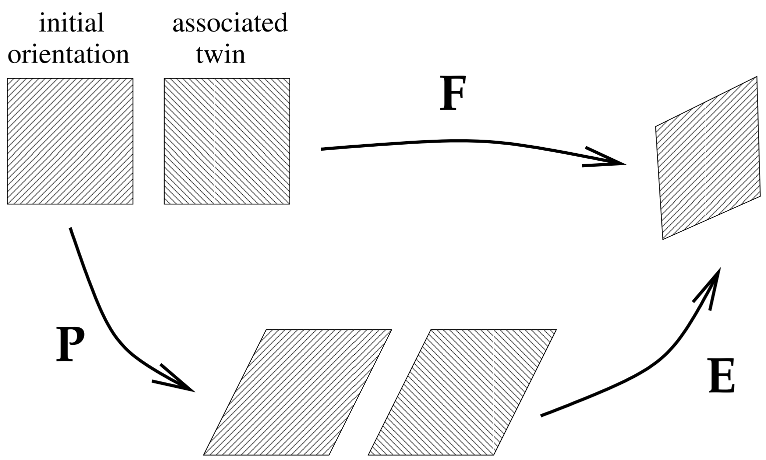

Figure 3: Kinematics of twinning plasticity

2.3. Thermodynamic setting

The state variables of the system can be taken as the Green–Lagrange strain tensor with respect to the intermediate configuration $\sharp$:

$$^{\sharp}\underset{\sim}{\Delta} = \frac{1}{2}(\underset{\sim}{\mathbf{E}}^T \underset{\sim}{\mathbf{E}} - \underset{\sim}{\mathbf{1}})$$

and temperature. The free energy $\psi(^{\sharp}\underset{\sim}{\Delta}, \alpha)$ may also be a function of an internal variable α to be specified. In the sequel, it is referred to the pure isothermal case. Only one twinning system is considered for simplicity. The local form of the energy balance equations then reads:

$$\rho\dot{\epsilon} = \underset{\sim}{\mathbf{T}} : \underset{\sim}{\dot{\mathbf{F}}}\underset{\sim}{\mathbf{F}}^{-1}$$

where $\underset{\sim}{\mathbf{T}}$ is the Cauchy stress tensor and ϵ the internal energy. The free energy takes the form:

$$\rho_\sharp\psi({}^\sharp\underset{\sim}{\Delta}, \alpha) = \frac{1}{2}\,{}^\sharp\underset{\sim}{\Delta} : \underset{\approx}{\mathbf{C}} : {}^\sharp\underset{\sim}{\Delta} + g(\alpha)$$

The Clausius–Duhem inequality reads:

$$-\rho_\sharp\dot{\psi} + \underset{\sim}{\mathbf{T}} : \underset{\sim}{\dot{\mathbf{F}}}\underset{\sim}{\mathbf{F}}^{-1} \geq 0$$

Noting that

$$\underset{\sim}{\mathbf{T}} : \underset{\sim}{\dot{\mathbf{F}}}\underset{\sim}{\mathbf{F}}^{-1} = (\underset{\sim}{\mathbf{E}}\underset{\sim}{\mathbf{T}}\underset{\sim}{\mathbf{E}}^{-T}) : \underset{\sim}{\dot{\mathbf{P}}}\underset{\sim}{\mathbf{P}}^{-1} + (\underset{\sim}{\mathbf{E}}^{-1}\underset{\sim}{\mathbf{T}}\underset{\sim}{\mathbf{E}}^{-T}) : {}^\sharp\underset{\sim}{\dot{\Delta}}$$

it follows that

$$-(\rho\frac{\partial\psi}{\partial\,{}^\sharp\underset{\sim}{\Delta}} - \underset{\sim}{\mathbf{E}}^{-1}\underset{\sim}{\mathbf{T}}\underset{\sim}{\mathbf{E}}^{-T}) : {}^\sharp\underset{\sim}{\dot{\Delta}} + (\underset{\sim}{\mathbf{E}}\underset{\sim}{\mathbf{T}}\underset{\sim}{\mathbf{E}}^{-T}) : \underset{\sim}{\dot{\mathbf{P}}}\underset{\sim}{\mathbf{P}}^{-1} - \rho\frac{\partial\psi}{\partial\alpha}\dot{\alpha} \geq 0$$

from which the state laws are deduced:

$${}^\sharp\underset{\sim}{\mathbf{T}} = \rho_\sharp\frac{\partial\psi}{\partial\,{}^\sharp\underset{\sim}{\Delta}} = \frac{\rho_\sharp}{\rho}\underset{\sim}{\mathbf{E}}^{-1}\underset{\sim}{\mathbf{T}}\underset{\sim}{\mathbf{E}}^{-T}$$

The thermodynamic force associated with the internal variable is:

$$A = -\rho_\sharp\frac{\partial\psi}{\partial\alpha} = -g'$$

The intrinsic dissipation rate then becomes:

$$D = {}^\sharp\underset{\sim}{\mathbf{S}} : \underset{\sim}{\dot{\mathbf{P}}}\underset{\sim}{\mathbf{P}}^{-1} + A\dot{\alpha}, \quad \text{with} \quad {}^\sharp\underset{\sim}{\mathbf{S}} = \frac{\rho_\sharp}{\rho}\underset{\sim}{\mathbf{E}}^T\underset{\sim}{\mathbf{T}}\underset{\sim}{\mathbf{E}}^{-T} = \underset{\sim}{\mathbf{E}}^T\underset{\sim}{\mathbf{E}}\,{}^\sharp\underset{\sim}{\mathbf{T}}$$

The positiveness of the intrinsic dissipation is then ensured by the choice of a convex dissipation potential $\Omega({}^\sharp\underset{\sim}{\mathbf{S}}, A)$:

$$\Omega({}^\sharp\underset{\sim}{\mathbf{S}}, A) = \frac{1}{n+1} < \frac{\tau - \tau_c}{K} >^{n+1}, \quad \text{with} \quad \tau = {}^\sharp\underset{\sim}{\mathbf{S}} : (\underline{\mathbf{m}} \otimes \underline{\mathbf{n}})$$

such that

$$\underset{\sim}{\dot{\mathbf{P}}}\underset{\sim}{\mathbf{P}}^{-1} = \frac{\partial\Omega}{\partial\,{}^\sharp\underset{\sim}{\mathbf{S}}} =< \frac{\tau - \tau_c}{K} >^n \ \underline{\mathbf{m}} \otimes \underline{\mathbf{n}}$$

$$\dot{\alpha} = \frac{\partial\Omega}{\partial A} = -\dot{\gamma}\frac{\partial\tau_c}{\partial A}$$

(1) $$D = \tau\dot{\gamma} + A\dot{\alpha}$$

Only calorimetric measurements can lead to an estimation of the dissipation associated with twinning in a single crystal. It appears from (1) that the amount of dissipated power is determined by the proper choice of the internal variable α and this will be dictated by the experimental measurements. Let us distinguish three cases:

• if no internal variable is introduced, $D = \tau\dot{\gamma}$ so that the entire plastic power is dissipated into heat; it is positive for a proper choice of $\underline{\mathbf{m}}$ and $\underline{\mathbf{n}}$ (such that $\tau > 0$ when $\dot{\gamma} > 0$), even if a softening behaviour is introduced;

• if we take $g' = \tau_c = -A$, then $\alpha = \gamma$ and $D = (\tau - \tau_c)\dot{\gamma}$ which vanishes in the rate-independent case; accordingly, the entire plastic power is considered as irreversibly stored, like dislocation forest hardening in dislocation–glide plasticity;

• if we take $\tau_c = \tau_0 - A$, i.e. $g' = -A = Q(1 - e^{-b\gamma})$, then $\alpha = \gamma$ and $D = (\tau - (\tau_c - \tau_0))\dot{\gamma} \simeq \tau_0\dot{\gamma}$ in the quasi–rate–independent case; it is again positive since the twinning system orientation convention is such that $\dot{\gamma} \geq 0$. This choice is classical in conventional elastoviscoplasticity ([1]).

A much more fine tuning of the internal variable will be necessary in the case of twinning ([17]) and is not undertaken here.

3. Finite element simulations of twinning in single crystals

The ability of the model to reproduce several experimental features of deformation twinning in single crystals is illustrated for three different situations. For that purpose, finite element simulations are provided based on classical nonlinear algorithms for the resolution of global equilibrium and the local integration of the evolution equations.

3.1. Twinning and untwinning under cyclic loading

The main justification for choosing a softening stress-strain constitutive equation in the model stems from the experimental results obtained by Price ([15]) on zinc whiskers deformed in tension under a transmission electron microscope. He was able to observe and control the nucleation of a single twin and its propagation in the sample cross–section. The twin then thickens and invades the entire specimen. The load–displacement curve displays a sharp softening stage associated with twin nucleation. The parameters of the model have been adjusted according to this curve.

The simulation of a single crystal zinc plate oriented for plane single twinning in tension is now considered. A geometrical defect is introduced to trigger strain localization that is interpreted here as twin nucleation. Indeed a deformation band appears and its orientation corresponds to that of a twin. Once the critical amount of shear γ_0 is reached, the twin starts growing. Twin growths is the result of the motion of the localization front on one or both sides of the twin in the spirit of ([12]). The twin thickens and spreads over the entire specimen (figure 5a). When the whole sample has twinned, the crystal behaves elastically in tension. The crystal can then be entirely untwinned if it is subsequently subjected to compression (figure 5b). It must be noted that at the last deformation stage, a virgin crystal is obtained that can again twin in tension. This results in the hysteresis loop shown in figure 4.

3.2. Twinning modes at a crack tip

Let us now consider a single crystalline Compact Tension specimen classically used in fracture mechanics. The $\underline{\mathbf{c}}$–axis of the zinc crystal is normal to the crack plane and the initial crack growth direction coincides with $[01\bar{1}0]$. It is recalled that twinning occurs in a specific direction η_1 and not in the opposite direction. A positive resolved shear stress in this direction is necessary for twinning to become possible. The distribution of resolved shear stresses for the single considered

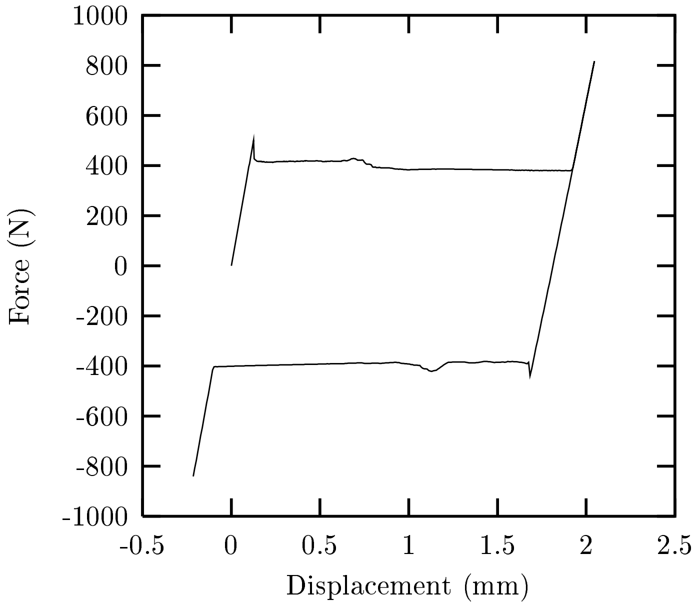

Figure 4: Load-displacement curve of the twinning and untwinning of a single crystal in tension-compression

twin system is shown on figure 6a. It appears that for the chosen orientation the resolved shear stress is negative ahead of the crack tip. Accordingly, a twin can form only behind the crack tip where the stresses are compressive. This is indeed possible as shown on figure 6b. This situation has been observed very often in the deformation of zinc coatings and is therefore justified by the present computation ([13]).

3.3. Multiple twinning in a zinc coating

The last example deals with the simulation of the formation of twin networks in a single crystal coating on an isotropic hyperelastic substrate subjected to tension. Two twinning systems are taken into account here: $[0\bar{1}1\bar{1}]$, $(0\bar{1}12)$ and $[01\bar{1}\bar{1}]$, $(01\bar{1}2)$. The $\underline{\mathbf{c}}$–axis of the crystal is normal to the coating and the tensile vertical direction is $[01\bar{1}0]$, parallel to the interface. The twinning directions of the considered systems are contained in the plane of the two–dimensional simulation. A displacement is prescribed at the top of the sample and the specimen is fixed at the bottom. Figure 7 shows that a first twin forms and is repelled at the interface, which corresponds to the formation of a second twin. A second pair of twins forms then independently at the lower part of the sample. Two of the twins intersect. The growth of the twins is limited by the fact that the interface cannot accommodate the deformation since the substrate remains elastic. Instead many twins form to build an actual network. This type of network is similar to that of figure 2. Sections of the coating are presented on figure 8 showing the twin development in the thickness of the coating. No direct experimental evidence of twin reflexion at the interface has been detected but this may be due to the specific crystal orientations.

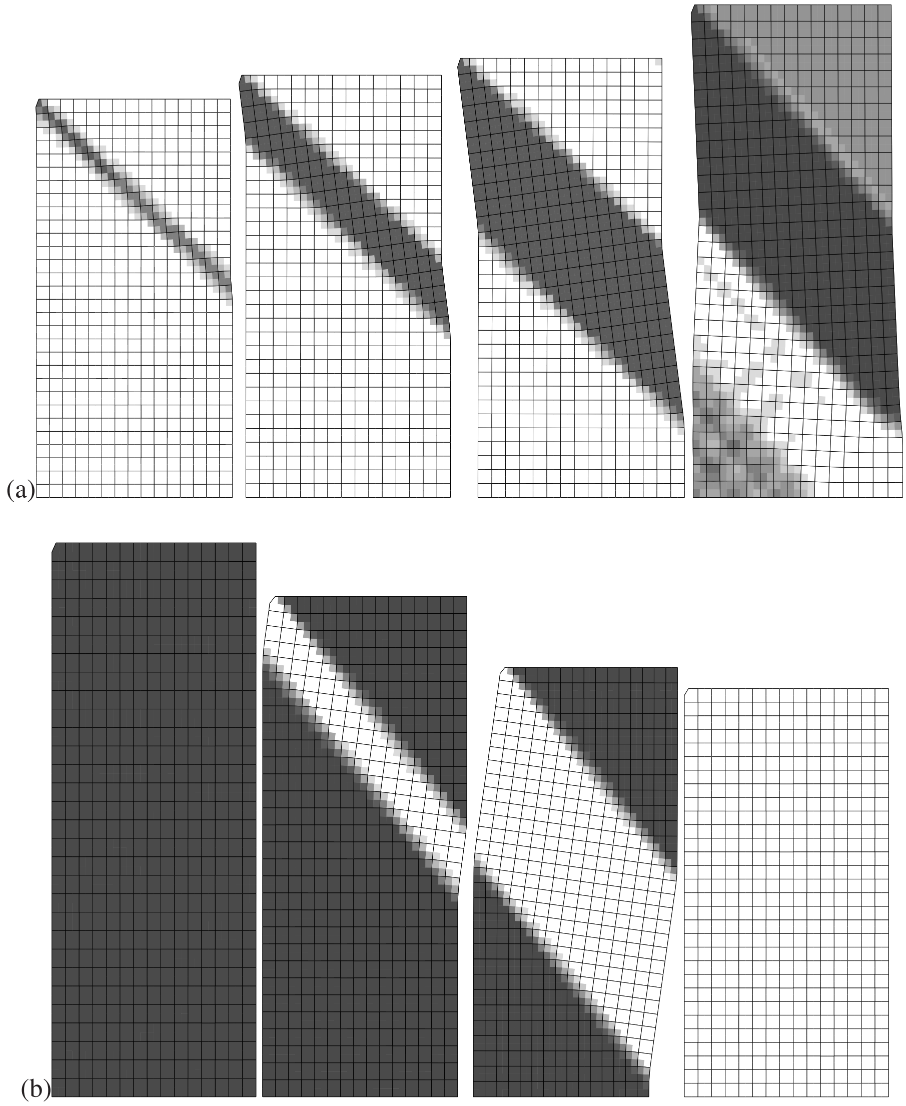

Figure 5: Twin formation and propagation in a single crystal in tension (a) followed by compression (b).

The twin systems activated in each strain localization band are given on figure 9. In the computation, the orientation of the sample is sligthly tilted with respect to the previously given orientation so that twin system 1 is significantly more activated than twin system 2. It is however quite surprising to see that the pair of almost perpendicular bands at the top of the sample belongs to the same twin system. This should in principle be impossible since two twins having the

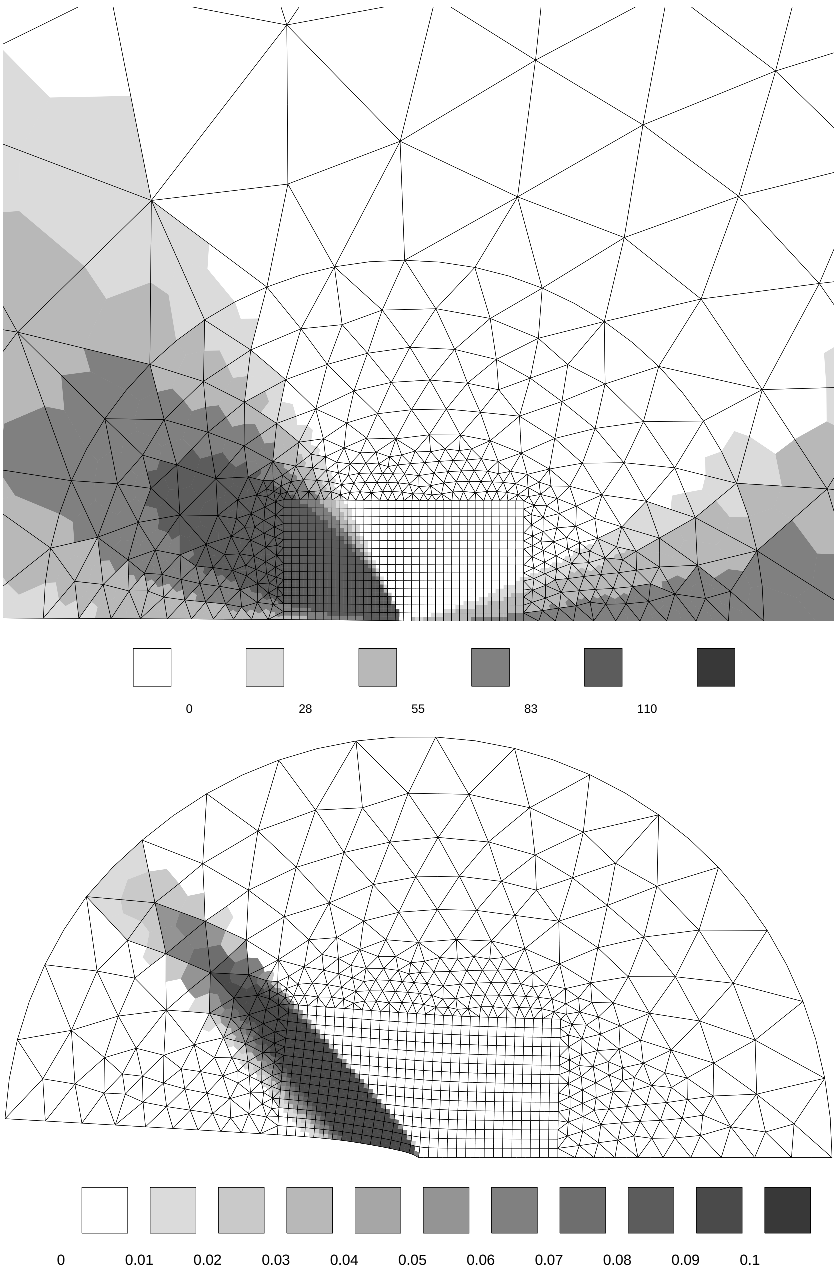

Figure 6: Twin formation at a cleavage crack tip : resolved shear stress distribution ((a), in MPa) and equivalent plastic deformation field (b).

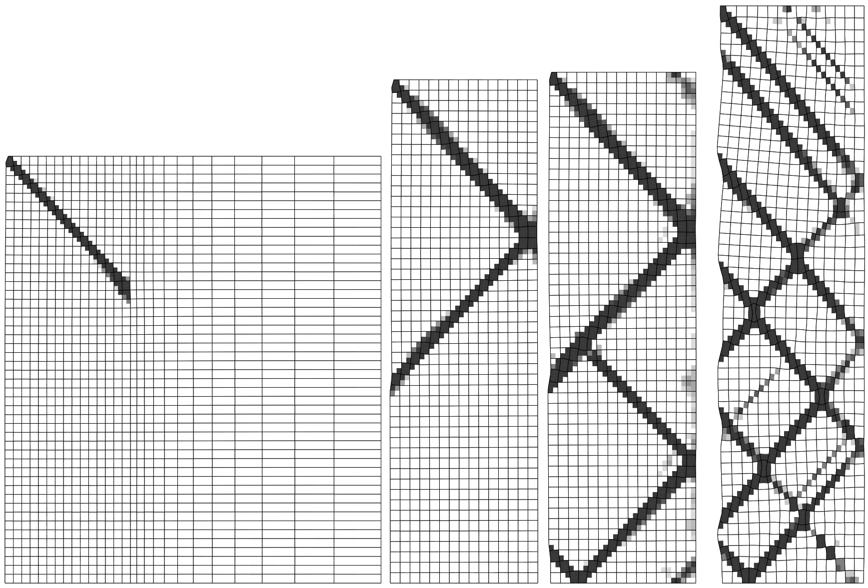

Figure 7: Multiple twinning in a zinc coating: the first twin is repelled at the interface coating/substrate (left), multiple reflexion and formation lead to a network of twins in the coating (right, only the coating is represented).

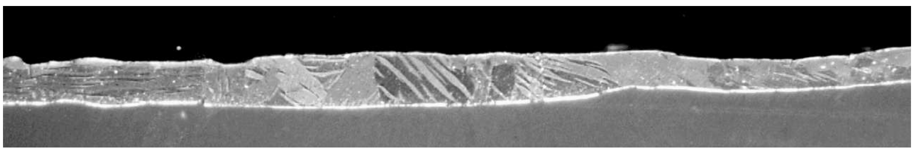

Figure 8: Section of the coating in the thickness showing the shape and orientation of the twins; the thickness of the coating is 10μm.

same twin plane should be parallel. These bands must be interpreted in fact as shear bands in a single crystal undergoing single slip. Simple glide in the twinning direction has been artificially introduced in the modelling to simulate twin formation. Twin formation has been interpreted as a strain localization phenomenon. In single slip, it is known that two localization planes are possible : slip bands lying in the slip plane but also kink bands that are normal to the slip direction ([5]). The last picture gives the distribution of lattice rotation with respect to the initial orientation before the twinned lattice has been reindexed. This information enables us in fact to distinguish the different types of bands : slip bands are usually associated with no lattice rotation whereas kink banding induces lattice curvature. It appears that the first twin at the top is a *kink twin* and the second one a "slip twin". A "kink twin" can be seen as a stacking of many parallel twin lamellae. A severe limitation of the model is that such kink twins are usually not observed experimentally.

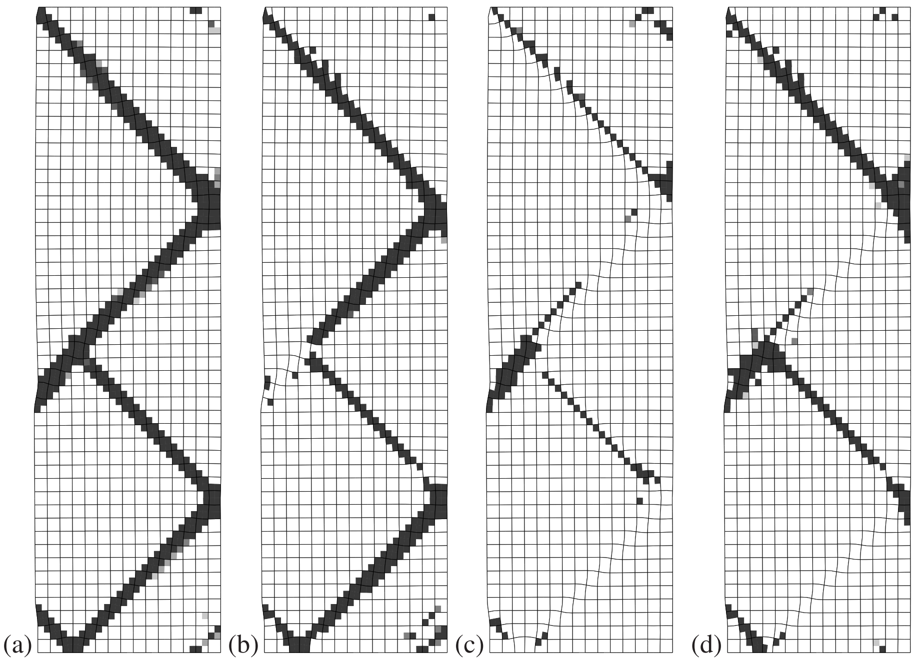

Figure 9: Structure of the twins in the coating : (a) equivalent plastic deformation, (b) twinning system 1, (c) twinning system 2, (d) lattice rotation before reindexing.

4. Discussion: The pros and the cons of the model

The proposed finite strain elastoplastic model of deformation twinning is able to account for several experimental features : twin formation and propagation in a single crystal, hysteresis loop associated with a twinning–untwinning process, arrow shape of twins at a cleavage crack tip and build–up of twin networks in a coating on a substrate.

Several important limitations remain however. One may for instance discuss the fact that a twinning criterion based on a critical resolved shear stress has been chosen. It is often recalled that twin initiation is a nucleation (in contrast to propagation) controlled process. It can therefore be affected for instance by prior dislocation glide so that it may be difficult to assign a critical value τ_0 to the twinning mechanism. Let us then admit that τ_0 is the critical resolved shear stress for twinning in a dislocation–free crystal like Price's zinc whiskers. The effective twin nucleation stress can then decrease if dislocation glide has already taken place, according to a softening law like:

$$\tau = \tau_0 + Q_2(1 - e^{-b_2 \gamma_{slip}})$$

where Q_2 is negative and γ_{slip} denotes the cumulative amount of prior dislocation glide.

Furthermore, deformation twinning is systematically associated with dislocation glide because of the high local stresses arising for instance at the twin tip. This interaction has not been taken into account yet, which leads to unrealistic local high stresses. Plastic slip can take place before twinning and the question to be solved is then : what happens to the obtained dislocation structure when it twins? How can prior slip activity affect further dislocation glide within the newly formed twin? Mechanical metallurgy has already provided some answers that must be incorporated into continuum modelling.

Special attention should also be paid to the intersection of twins that has occured in some simulations.

A strong limitation has already been pointed out, namely the prediction of kink twins that are not observed in practise. The elimination of such deformation modes is however possible using for instance Cosserat crystal plasticity ([6, 7]).

An alternative approach to deformation twinning is proposed in ([8]) based on minimization principles. This global approach enables one to predict self–equilibrating structures that are frequently observed. The difficulty then is the numerical exploration of all possible regions and shapes where twinning can occur in order to finger out the most favourable configuration. The authors themselves plead for a Landau–Ginzburg or Cahn–Hilliard–type of modelling of displacives phase transitions and deformation twinning. That is why an improvement of the present model could be the introduction of an order parameter, aiming at forbiding "interrupted twins", i.e. regions where crystal glide has begun but where the value γ_0 has not been reached yet.

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