Microscale Modelling of Higher Order Deformation Twinning

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Introduction. Many industries such as aircraft, automotive or direct steel companies extensively use metals like TWIP steels, Ti, Mg, Zr, etc. The key factors of their deformation mechanisms are deformation twinning and crystallographic slip. The twinning is an intriguing and unavoidable phenomenon during deformation. However, the modelling of higher order twinning on the grain scale is still missing. We model the higher order twinning of crystals of lower symmetries by minimizing the elastic strain energy. The model can successfully predict the nucleation and the propagation of the twinning on the grain scale in order to understand the underlying physics of high ductility and large elongation of metals. So far, this is the first of this kind that predicts higher order twin nucleation and propagation on the grain scale.

Problem Definition

The minimum elastic strain energy (MESE) approach has been implemented since a system always stays at a minimum energy level. 12 (for Ti) twin variants are defined in total with respect to the reference placement and stress free configurations including the possibility of de-twinning

Objectives

1. To model the initiation and propagation of higher order deformation twinning on the grain scale
2. To identify the truly activated twinning mode
3. To incorporate the change of stress free placements

Cooperation

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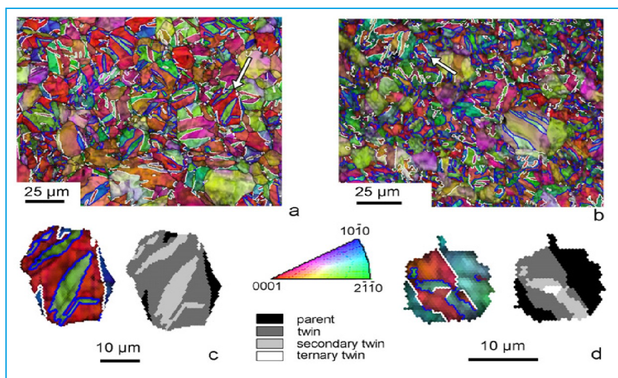
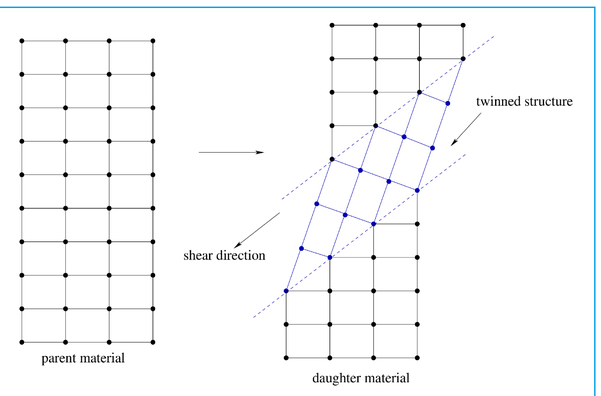
Prof. Thorsten Halle, Institut für Werkstoff- und Fügetechnik (IWF), Magdeburg
Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf

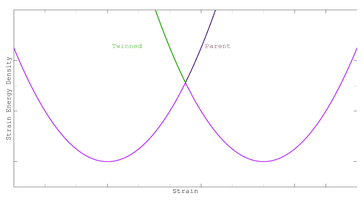
Experiment and Model Setup



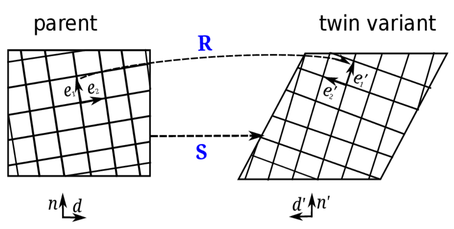
Micrographs of Ti: higher order twinning (W. Tirry et al. 2011)



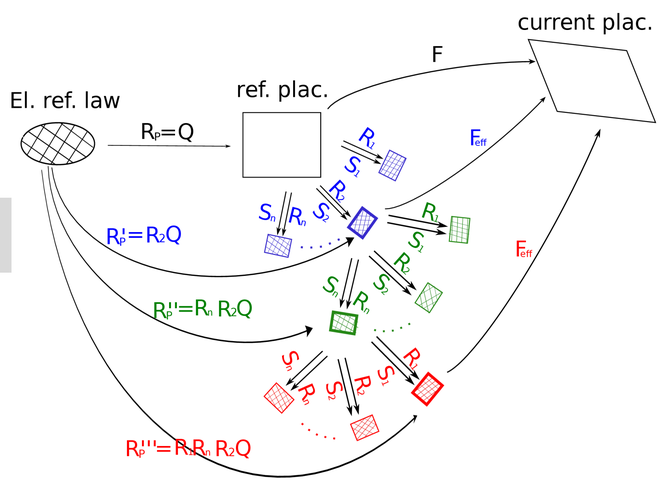
Schematic diagram of deformation twinning



The minimum elastic energy approach



At least two transformation are required to define twinning



Modelling approach: the successive updating mechanism

Analytical Description

Green's strain tensor $\mathbf{E} = \frac{1}{2}(\mathbf{C} - \mathbf{I}), \mathbf{C} = \mathbf{F}^{\mathrm{T}}\mathbf{F}$

Elastic reference strain energy density

$$w_0(\mathbf{C}) = \frac{1}{2}\mathbf{T}^{2\mathrm{PK}} : \mathbf{E} = \frac{1}{8}(\mathbf{C} - \mathbf{I}) : \mathbb{K} : (\mathbf{C} - \mathbf{I})$$

$\mathbb{K}$ is the material stiffness tensor

Twinning is isomorphic, hence, the elastic energy density of i^{th} variant $w_i(\mathbf{C}) = w_0(\mathbf{P}_i^{\mathrm{T}}\mathbf{C}\mathbf{P}_i)$ $\mathbf{P}_i = \mathbf{S}_i^{-1}\mathbf{R}_i$

$\mathbf{R}_i$ is the crystal orientation,
$\mathbf{S}_i$ is the shear deformation corresponding to the i^{th} variant

2nd Piola-Kirchhoff stress tensor of i^{th} variant

$$\mathbf{T}_i^{2\mathrm{PK}} = \frac{\partial w_i(\mathbf{C})}{\partial \mathbf{E}} = 2\frac{\partial w_i(\mathbf{C})}{\partial \mathbf{C}} = 2\mathbf{P}_i w_0'(\mathbf{P}_i^{\mathrm{T}}\mathbf{C}\mathbf{P}_i)\mathbf{P}_i^{\mathrm{T}}$$

2nd Piola-Kirchhoff stress tensor because of MESE approach

$$\tilde{\mathbf{T}}^{2\mathrm{PK}} = \frac{\partial \tilde{w}(\mathbf{C})}{\partial \mathbf{E}} = 2\tilde{\mathbf{P}} w_0'(\tilde{\mathbf{P}}^{\mathrm{T}}\mathbf{C}\tilde{\mathbf{P}})\tilde{\mathbf{P}}^{\mathrm{T}}$$

Viscous relaxation scheme is used $\mathbf{T}^{2\mathrm{PK}} = \tilde{\mathbf{T}}^{2\mathrm{PK}} + \eta\dot{\mathbf{E}}$
η is the viscosity parameter

Projection criterion: $\gamma_i = \mathbf{F}^{\mathrm{eff}} : (\mathbf{d}_i \otimes \mathbf{n}_i), \qquad i = 1, \ldots, n$
Where $\mathbf{d}_i$ and $\mathbf{n}_i$ are the twin direction and twin normal of i^{th} variant

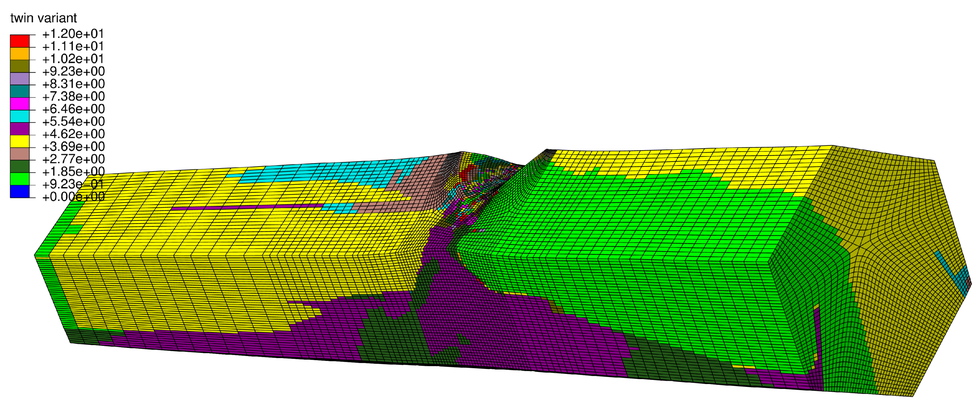


Fig. 2: Simulation on the single crystal of Ti by ABAQUS. Multiple twin systems are activated in a deformation controlled tensile test

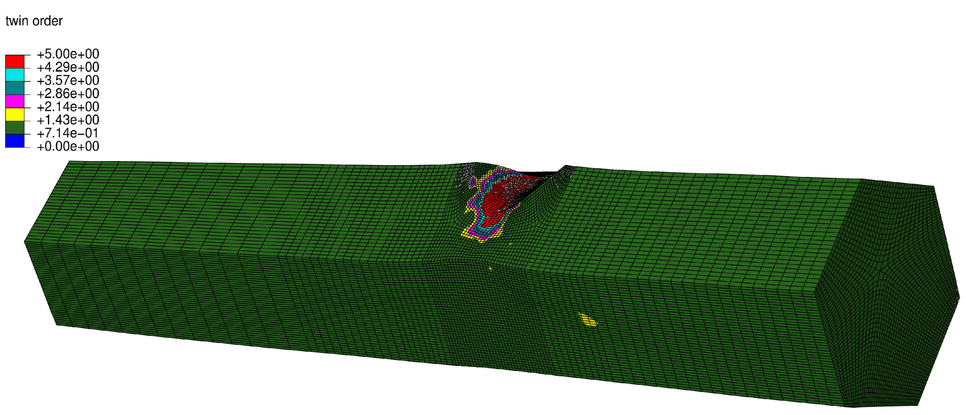


Fig. 1: Simulation on the single crystal of Ti. Higher order (5 in total) twinning in a deformation controlled test.

Results and Discussion

the higher order twinning is observed in the single crystal computational experiment for Ti (Fig. 1)
the multiple twin systems are activated in any order of twinning (Fig. 2)
the twin thickness is large and the whole sample can be transformed to twinned material (Fig. 2)

the model is limited to the thick twins like twins in the crystals of lower symmetry
the kinetics of interface is roughly predictable only by bulk viscosity
overestimated stress-level; stress-adaptation comes with drawbacks

Conclusions

1. A kinematic framework of multiple and higher order twinning is established.
2. A projection criterion is used to identify the preferred twinning mode.
3. The model successfully predicts twin nucleation and propagation on the grain scale.
4. The model successfully predicts the crystal reorientation and grain refinement
5. It can be applicable to any hcp materials that show twinning
6.The model has only two control parameters, one for the viscosity and second for the regularization
7. Extension on the twin migration across grain boundary (GB) and interaction with GB can lead to investigate its effect in polycrystal

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