FTMP-based Modeling and Simulation of Magnesium

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Abstract

The present study proposes a constitutive model for deformation twinning which taking account of the twin degrees of freedom via incompatibility tensor model based on Field Theory of Multiscale Plasticity (FTMP). The model is introduced in the hardening law in the FTMP-based crystalline plasticity framework, which is further implemented into a finite element code. Deformation analyses are made for pure single crystal magnesium with HCP structure, and the descriptive capabilities of the proposed model are confirmed based on critical comparisons with experimental data under plain-strain compression in multiple orientations, available in the literature. The simulated results are demonstrated to successfully reproduce the unique stress-strain responses induced by twinning. The evolution of the relative activities of the various slips, and twin mechanisms for each orientation are extensively examined.

Keywords: Deformation twinning, Crystalline plasticity, Multiscale modeling, Field theory, Magnesium

Introduction

The extensive use of Mg in industry has attracted many attentions in recent years mainly because of its superior properties such as light-weight, high strength, and workability. Specifically, unfavorable textures inevitably introduced during rolling processes tend to inhibit both deformability and formability of the material. Therefore, intensive studies have been conducted by many researchers aiming at appropriately controlling the textures. Moreover, complicated fracture modes are observed such as cracking along twin boundaries where twin-slip/twin-twin interactions take place. Accordingly, subtle balances among the different degrees of freedom result in distinct stress-strain responses. A tangible of example of making positive use of such feature is the addition of Yttrium (Nagao, 2012): Yttrium tends to inhibit the twin boundary cracking that leads effectively to the enhancement of the ductility (elongation), thereby relaxing the stress concentration, which is consumed via sub-grain formations or else rotations about the c-axis. What we learn from such observed facts is not only the twin degrees of freedom but also the others associated with all the possible mechanisms ought to be appropriately taken into account in the proposed model.

A key to establish a successful model for Mg is undoubtedly the rational modeling of the deformation twinning in the above-mentioned respect. Major difficulties of the twin modeling come down to how to express the twinning degrees of freedom as an alternative to the slip-based deformation in rational as well as sophisticated manners. A simple but robust model proposed by van-Houtte (van-Houtte, 1978) has been widely used in simulating twin-related phenomena, partially because of its conciseness in the implementation into the conventional crystal plasticity framework. The descriptive capabilities of the model, however, are evidently limited, in the sense that the model will unable to simulate, e.g., the above-mentioned experimental observation.

Hasebe have advocated a comprehensive theoretical framework and model named Field Theory of Multiscale Plasticity (FTMP) (Hasebe, 2004, 2006) that is effective for tackling the above issues. In FTMP, differential geometric quantities, i.e., curvature and torsion, are utilized to rationally describe the generalized "inhomogeneity." The theory provides us with general views concerning not only how we should recognize the elasto-plastic hierarchy in terms of "evolving" inhomogeneities but also how we can model the targeted phenomena in terms of underlying microscopic degrees of freedom within, e.g., crystal plasticity-based continuum mechanics framework. Geometrically-necessary types of dislocation substructures, as examples of slip-induced inhomogeneities, have demonstrated to be successfully reproduced based on the model (Aoyagi and Hasebe, 2007; Tsunemi and Hasebe, 2009; Imiya and Hasebe, 2013). The model is also applied to the twin modeling and simulations (Okuda and Hasebe, 2013).

In this paper, we apply the FTMP-based model for deformation twinning to Magnesium (Mg, hereafter) with HCP (hexagonal close-packed) structure. Based on the kinematic descriptions for HCP metals, i.e., with the three slip systems (basal, pyramidal and prismatic) and two twin systems (tensile/compression twins), the proposed model will be applied to Mg. The basic capabilities for pure Mg (with mechanical properties available in the literature) will be examined.

Theoretical Background and Model for Deformation Twin

Differential Geometrical Pictures of Dislocation/Defect Fields

The theory (FTMP) partially puts its basis on the differential geometrical descriptions of dislocations and defects. The major concepts have been established as non-Riemannian plasticity by Kondo (Kondo, 1955). Here, some basics are outlined.

Torsion and curvature tensors are defined, as shown above, respectively as,

$$\begin{cases} S_{kl}^{\cdot\cdot j} = \Gamma_{[kl]}^{j} \\ R_{klm}^{\cdots n} = 2\left[\partial_{[k} \Gamma_{l]m}^{n} + \Gamma_{[k|p|}^{n} \Gamma_{l]m}^{p} \right] \end{cases} \tag{1}$$

where Γ_{kl}^{j} represents the coefficients of connection Γ_{kl}^{j} in the non-Riemannian space.

Contractions of these higher order tensors considering the symmetry result in well-known second rank tensors. They are respectively called "dislocation density tensor" and "incompatibility tensor" given respectively by a curl of distortion tensor and double curl of strain tensor, i.e.,

$$\begin{cases} \alpha_{ij} = -\in_{ikl} \partial_k \beta_{lj}^{p} = \frac{1}{2} \in_{ikl} S_{kl}^{\cdot\cdot j} \\ \eta_{ij} = \in_{ikl} \in_{jmn} \partial_k \partial_m \varepsilon_{ln}^{p} = \dfrac{1}{4g} \in_{ikl} \in_{jmn} R_{klm}^{\cdots n} \quad (g = \det(g_{ij})) \end{cases} \tag{2}$$

To be noted that these quantities are expressed as gradients of distortion or strain tensor in the context of continuum mechanics, meaning the theory intrinsically requires "strain gradients" at least up to the second order.

Modeling Deformation Twin – Kinematics and Constitutive Model

The constitutive models both for slip and deformation twinning employed in the present study are overviewed. Here, the elasto-plastic decomposition by Lee is extended to that including the twin deformation by introducing an intermediate configuration,

$$\boldsymbol{F} = \boldsymbol{F}^e \cdot \boldsymbol{F}^{tw} \cdot \boldsymbol{F}^p \tag{3}$$

where the deformation gradient tensor for the twinning is represented by F^{twin}. Correspondingly, the Jaumann rate of the Kirchhoff stress tensor is given by,

$$\boldsymbol{\tau}_{(J)} = \boldsymbol{C}^e : \boldsymbol{d} - \sum_{\alpha=1}^{N} \boldsymbol{R}^{(\alpha)} \dot{\gamma}^{(\alpha)} + \sum_{\bar{\alpha}=1}^{N} \boldsymbol{R}^{tw(\bar{\alpha})} \dot{\gamma}^{tw(\bar{\alpha})} \qquad (4)_1$$

with

$$\begin{cases} \boldsymbol{R}^{(\alpha)} = \boldsymbol{C}^e : \boldsymbol{P}^{(\alpha)} + \boldsymbol{\beta}^{(\alpha)} \\ \boldsymbol{\beta}^{(\alpha)} = \boldsymbol{W}^{(\alpha)} \cdot \boldsymbol{\sigma} - \boldsymbol{\sigma} \cdot \boldsymbol{W}^{(\alpha)} \end{cases} \text{and} \begin{cases} \boldsymbol{R}^{tw(\bar{\alpha})} = \boldsymbol{C}^e : \boldsymbol{P}^{tw(\bar{\alpha})} + \boldsymbol{\beta}^{tw(\bar{\alpha})} \\ \boldsymbol{\beta}^{tw(\bar{\alpha})} = \boldsymbol{W}^{tw(\bar{\alpha})} \cdot \boldsymbol{\sigma} - \boldsymbol{\sigma} \cdot \boldsymbol{W}^{tw(\bar{\alpha})} \end{cases} \qquad (4)_2$$

The slip rate is given by,

$$\begin{cases} \dot{\gamma}^{(\alpha)} = \dot{A}_{SR} sgn(\tau^{(\alpha)}) \left\{ exp\ B_{SR} \left(1.0 - \left| \dfrac{\tau^{(\alpha)}}{K^{(\alpha)}} \right|^p \right)^q + C_{SR} \right\}^{-1} \\ \dot{A}_{SR} = \rho_m b L \nu_0\ , \qquad B_{SR} = \dfrac{\Delta G_0}{kT}\ , \qquad C_{SR} = \dfrac{\nu_0 BL}{K^{(\alpha)}} \end{cases} \tag{5}$$

where $K^{(\alpha)}$ is drag stress, responsible for isotropic type of hardening. The above constitutive equation can express stress-strain responses for FCC, HCP and BCC metals over a wide range of strain rate and temperature including impact loading conditions.

The evolution models for drag stress $K^{(\alpha)}$ and back stress $\Omega^{(\alpha)}$ given respectively by [Hasebe, Kumai and Imaida (1998b)],

$$\dot{K}^{(\alpha)} = Q_{\alpha\beta} H(\gamma) \left| \dot{\gamma}^{(\beta)} \right| \text{ and } \dot{\Omega}^{(\alpha)} = -A_{cell} \left\{ \left\langle d_{cell}^{*} - \bar{x}_N^{(\alpha)} \right\rangle + \alpha \right\}^{-2} \tag{6}$$

where $H(\gamma)$ represents hardening modulus for a referential stress-strain curve. The hardening ratio $Q_{\alpha\beta}$, through which the contributions of $\tilde{\alpha}^{(\alpha)}$ and $\tilde{\eta}^{(\alpha)}$ are accounted for, is given by,

$$Q_{\alpha\beta} = f_{\alpha\kappa} S_{\kappa\beta} + \delta_{\alpha\beta} \left\{ 1 + F\ (\tilde{\alpha}^{(\alpha)}; \tilde{\eta}^{(\alpha)}) \right\} \tag{7}$$

The strain gradient terms are given as,

$$F(\alpha^{(\alpha)}) = \frac{\bar{k}}{p_\alpha} \sqrt{\frac{\left|\alpha^{(\alpha)}\right|}{b}}\ , \quad F(\eta^{(\alpha)}) = \mathrm{sgn}(\eta^{(\alpha)}) \frac{\bar{k}}{p_\eta} \sqrt{\frac{l_{defect}}{b} \left|\eta^{(\alpha)}\right|} \tag{8}$$

where b denotes the Burgers vector and $\bar{k}$, p_α and p_η are the material constants. $\alpha^{(\alpha)}$ and $\eta^{(\alpha)}$ are respectively written in the forms as mappings of α_{ij} and η_{ij} into a α slip system.

The strain rate due to deformation twin is assumed to be an additional degree of freedom to that due to the slip, driven by the evolution of the incompatibility tensor field for the twinning mode, $\eta_{tw}^{(\bar{\beta})} \equiv \left(\boldsymbol{t}^{tw(\bar{\beta})} \otimes \boldsymbol{s}^{tw(\bar{\beta})} \right) : \boldsymbol{\eta}$, i.e.,

$$\dot{\gamma}^{tw(\bar{\alpha})} = Q_{\bar{\alpha}\bar{\beta}}^{tw} \left| \dot{\gamma}_{prev}^{tw(\bar{\beta})} \right|, Q_{\bar{\alpha}\bar{\beta}}^{tw} = \delta_{\bar{\alpha}\bar{\beta}} \cdot F\left(\eta_{tw}^{(\bar{\beta})}\right) \cdot \left\langle 1 - \frac{\left|F\left(\eta_{tw}^{(\bar{\beta})}\right)\right|}{F_{sat}^{tw}} \right\rangle \tag{9}$$

Here, $F\left(\eta_{twin}^{(\bar{\beta})}\right)$ denotes the FTMP-based incompatibility term defined as,

$$F\left(\eta_{twin}^{(\bar{\alpha})}\right) \equiv \mathrm{sgn}(\tilde{\eta}^{(\alpha)}) \cdot \frac{k}{p_\eta} \left(\frac{l_{twin}}{b} \left| \eta_{twin}^{(\bar{\alpha})} \right| \right)^{1/2} \tag{10}$$

The above twinning model becomes operative when the critical condition for the resolved shear stress is met, i.e., $\tau^{\chi} \geq \tau_{cr}^{t}$.

Analytical Model and Procedure

Deformation analyses are made for pure single crystal magnesium (Mg) with HCP structure, and the descriptive capabilities of the proposed model are confirmed based on critical comparisons with experimental data under plain-strain compression in multiple orientations, available in the literature (Kelley and Hosford, 1967, 1968).

Kelly-Hosford conducted a systematic series of plane-strain compression experiments on Mg single crystals, as schematically illustrated in Fig.1. In the present simulations, the die-constraint condition is realistically mimicked by using plane strain assumption. The orientations E and F are reported to exhibit peculiar stress responses showing plateau-like work hardening stagnation followed by a rapid stress increase. The plateau-like stress response observed for the two orientations is supposed to be an indication of the twin activity as the dominant deformation mode, while the latter (rapid stress increase) is driven by the outset of slip modes.

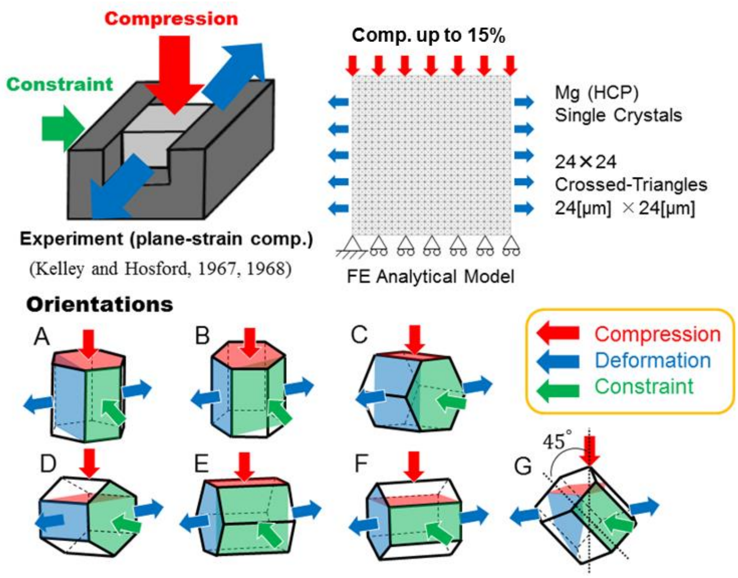

Figure 1. Simulation set-ups for plane-strain compressions of single crystal magnesium in various crystallographic orientations, where original experiments are conducted by Kelly-Hosford (1967, 1968). Twinning mode is reported to be dominantly activated in orientations E and F.

Results and Discussion

Orientation-dependent stress-strain responses

Figure 2 shows the simulated stress-strain curves for the A-G orientations, comparing with the experimental data (plots). We find excellent agreements between the two for all the orientations. In particular, the simulated results for orientations E and F are demonstrated to successfully reproduce the unique stress-strain responses induced by twinning.

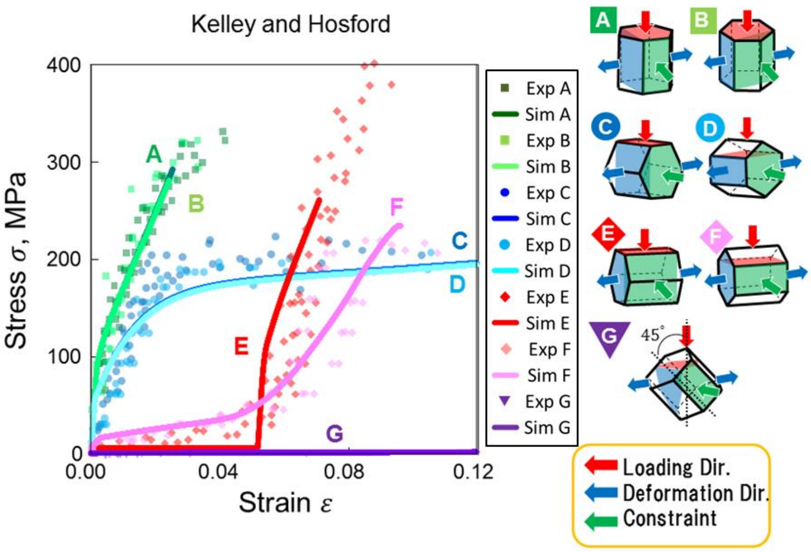

Figure 2. Simulated stress-strain curves for orientations A to G. Corresponding experimental data by Kelly-Hosford are overplotted for comparison.

Sample size dependence and Mesh size dependence

One of the noteworthy features of the present model is the ability to represent absolute scale that is conveyed through the evaluation range of spatial derivative for obtaining the incompatibility tensor field. For the orientations E and F where the twinning mode is dominant, we expect that the stress response is sensitively affected by the sample dimensions. Figure 3 (a) shows the variation of the stress-strain diagram with the sample size for the orientation E, while Fig.3 (b) displays the same result but for the orientation F. What can be clearly confirmed is that the emerging patterns obviously depend on the sample size both for the two orientations. The peculiar stress responses, i.e., plateau-like stress response due to the dominant twinning mode followed by the slip-induced rapid stress rise, are basically unaltered regardless of the sample size. Roughly, larger sample size tends to yield earlier outset of the stress rise, except orientation F with $12\times12\mu m^2$. The variation of the stress-strain curves roughly covers the scatter range of the data in the experiment both for the orientations E and F, implying a possible reason for causing the scatter in the real situations.

To examine the mode-wise contributions, we evaluate the activity ratio of the slip/twin modes for the two cases. Here, activity ratios among two twinning modes and three slip modes are considered, where the total contribution of all the modes is normalized to 1.

Figure 4 compares the variations of slip/twin activity ratio with strain among the three sample sizes for (a) orientation E and (b) orientation F. Orientation E yields 100% activity of the tensile twin mode until the pyramidal and prismatic slip modes are abruptly activated, when the twin activity is stagnated. This corresponds to the stress rise in Fig.3 (a). For orientation F, on the other hand, the prismatic slip is also active in addition to the tensile twin from the early stage of deformation, which lasts (or slightly increases) even after the twin activity is declined. When the activity of the tensile twin starts to be declined, the pyramidal slip is activated, similar to the trend in orientation E. An intriguing point to be noted here is the activity of the basal slip is found in the smallest sample size, $12x12\mu m^2$, which is absent in all the other cases. The smaller the sample size is, the more the boundary condition becomes influential on the subtle slip/twin activities within. The basal slip, in this case, tends to restrict the activities of the others, i.e., prismatic and the pyramidal slip modes.

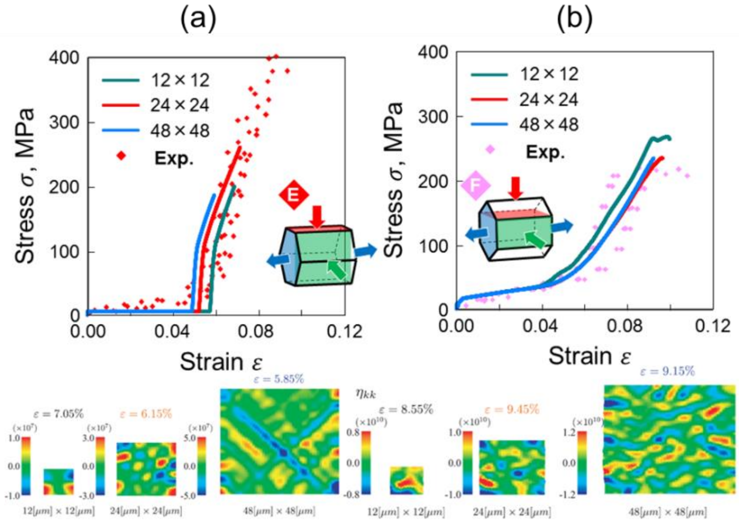

Figure 3. Sample size effect on emerging twinning pattern (strain contour) and stress-strain responses for orientations E and F, comparing 12×12, 24×24 and 48×48μm^2.

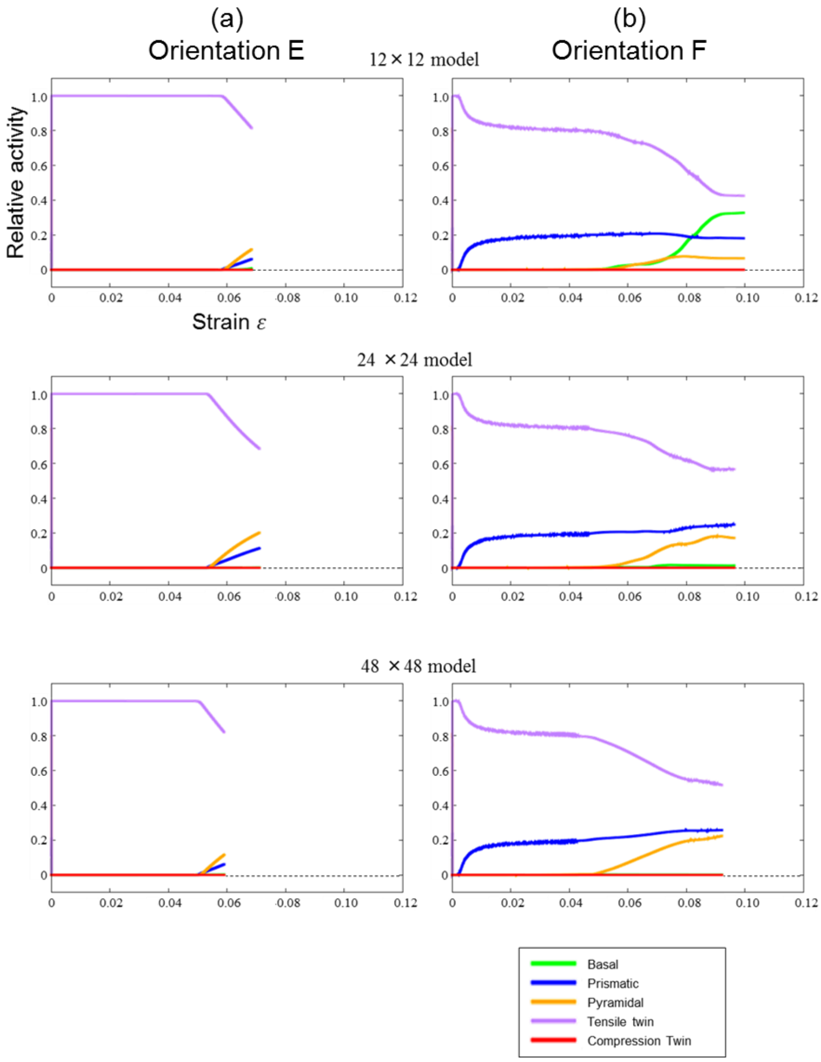

Figure 4. Relative activities of slip and twin modes depended orientation and analysis conditions, comparing three model sizes, i.e., 12x12, 24x24 and 48x48 μm^2.

Another feature to be noted of the current modeling scheme is its mesh independency of the simulation results. To demonstrate this, simulations using two mesh divisions, 24x24 and 48x48 cross triangle elements, with a common evaluation size of the derivative for the incompatibility tensor calculation, are compared. Figure 5 shows two twinning strain contours with different mesh divisions. One can confirm basically the same patterns regardless the mesh size. The corresponding stress-strain curves are displayed in the inset, showing almost identical response.

As leverage, let us briefly review conventionally-proposed models, pointing out their drawbacks. They in common introduced a sort of mode transition condition from twin to slip in artificial manners (e.g. Graff, Steglich and Brocks, 2007; Zhang and Josh, 2012). For example, Graff, et al. assumed two functions in their hardening law as,

$$h(\gamma) = \begin{cases} h_0 & \text{for } \gamma \le \gamma_{ref} \\ h_0 \left(\dfrac{\gamma}{\gamma_{ref}} \right)^{m-1} & \text{for } \gamma \ge \gamma_{ref} \end{cases} \tag{8}$$

As can be easily imagined, such models always behave similarly regardless of the sample geometry and dimensions, which is obviously unrealistic.

The phase field (PF) model, on the other hand, seems to be powerful even considering the above respect at first glance. We ought to notice, however, it requires us to introduce initial fluctuations in the phase field (twined region, in this case) that critically controls the nucleation site and number of the twined regions. Since where and when the twinning should take place varies strongly depend on the precursor inhomogeneities and other boundary conditions, the PF approach needs some rational reasoning for introducing the initial field fluctuations.

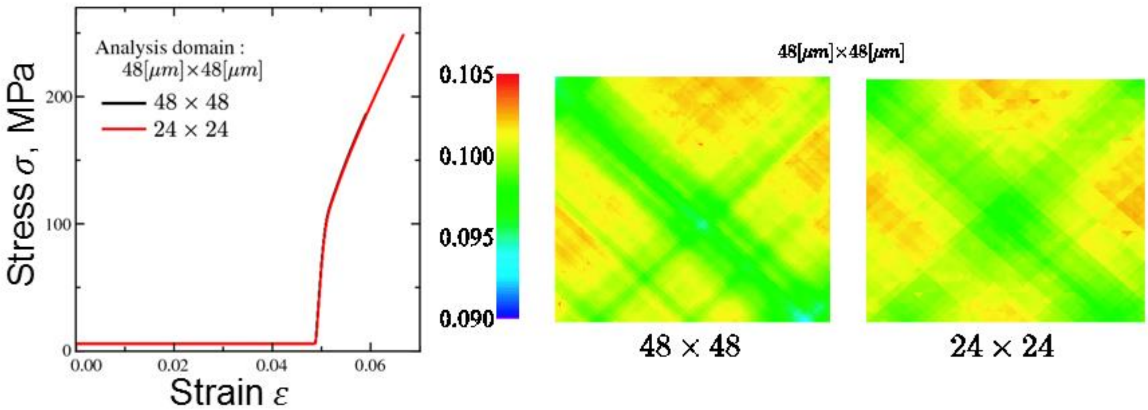

Figure 5. Supplementary results demonstrating mesh independency of proposed model-based simulations. Strain contours for twinning and corresponding stress-strain diagrams almost coincide regardless the mesh division.

Conclusion

A new rational model for deformation twinning has been developed, extending the original FTMP theory of Hasebe for dislocation-based crystal plasticity. Twinning degrees of freedom are taken into account via the FTMP-based incompatibility model, which is further implemented into a crystalline plasticity constitutive framework via the hardening law. Numerical simulations have been performed for pure single-crystal magnesium with HCP structure, and descriptive capabilities of the model have been confirmed by critical comparisons with experimental data for plane-strain compression of crystals of multiple orientations available in the literature. Results successfully reproduce the unique stress-strain responses induced by twinning. Activities of the various slip systems and twinning mechanisms for each orientation have been predicted. Other noteworthy features addressed here, but not captured by conventional continuum plasticity models, are sample size dependence and mesh size independence.

Acknowledgement

A support from Army Research Laboratory (ARL) under Contract No. FA5029-13-P-0043 is greatly acknowledged.

References

Aoyagi, Y. and Hasebe, T., (2007), New Physical Interpretation of Incompatibility Tensor and Its Application to Dislocation Substructure Evolution. *Key Materials Engineering*, 340-341, 217-222.

Graff, S., Steglich, D. and Brocks, W., (2007), Forming of Magnesium-Crystal Plasticity and Plastic Potentials. *Adv. Eng. Maters*., 9-9, 803-806.

Hasebe, T., (2006), Multiscale Crystal Plasticity Modeling based on Field Theory. *Comp. Mech. Eng. Sci.* (*CMES*), 11-3, 145-155.

Hasebe, T., (2004), Continuum Description of Inhomogeniously Deforming Polycrystalline Aggregate based on Field Theory. *Meso-Scale Simulation and Modeling of Strength and Fracture of Materials*, *IUTAM Symp. Mesoscopic Dynamics of Fracture Process and Materials Strength* (Eds. H. Kitagawa and Y. Shibutani), Kluwer, pp.381-390.

Hasebe, T., (2004), Field Theoretical Multiscale Modeling of Polycrystal Plasticity. *Trans. MRS-J*, Vol.29, pp.3619-3624.

Hasebe, T., (2011), Field Theory of Multiscale Plasticity. Cambridge (to be published).

Kelly, E. W. and Hosford, W. F. Jr., (1968), The Deformation Characteristics of Textured Magnesium. *Trans. Metall. Soc. AIME*, 242, 5; ibid. 242, 654.

Kondo, K. (1955), Non-Riemannian Geometry of Imperfect Crystals from a Macroscopic Viewpoint. *RAAG Memoirs of Unifying Study of Basic Problems in Engineering and Physical Science by Means of Geometry*, 1 D-I, 458-469.

Nagao, M., Mukai, T. and Somegawa, H., (2012), Ductility of Ma-Y binary alloy under dynamic compression loading. The 123nd Conference of Japan Institute of Light Metals, pp. 335-336.

van Houtte, P., (1978), Simulation of the Rolling and Shear Texture of Brass by the Taylor Theory Adapted for Mechanical Twinning. *Acta Metall*., 26, 591-601.

Zhang, J. and Josh, S. P., (2012), Phenomenological Crystal Plasticity Modeling and Detailed Micromechanical Investigations of Pure Magnesium. *J. Mech. Phys. Solids*, 60-5, 945-972.

Okuda, T., Imiya, K. and Hasebe, T., FTMP-based Simulation of Twin Nucleation and Substructure Evolution under Hypervelocity Impact. Graduation thesis, Kobe University.

Tsunemi, Y. and Hasebe, T., (2009), Simulation of the Heterogeneous Ground Development based on a Distortion Incline Model. Graduation thesis, Kobe University.

Imiya, K. and Hasebe, T., (2013), Modeling of Twin Deformation based on Field Theory of Multiscale Plasticity. Master's thesis, Kobe University.

Hasebe, T., Kumai, S. and Imaida, Y., (1998), Impact Compression Behavior of FCC Metals with Pre-Torsion Technique. J. Maters. Process. Technol., 85, 194-197.