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Constitutive Modeling based on Evolutionary Multi-junctions of Dislocations

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Abstract. A latent hardening model based on binary junction-induced hardening can effectively describe the anisotropy measured in multiaxial tests. However, this approach still has some descriptive and predictive limitations. Recent findings show that binary junctions generated by interactions of pairs of dislocations can only induce short-term hardening effect due to the unzipping process of binary junctions. By contrast, multi-junctions, which are formed via multiple interactions of dislocations, can exert a strong and enduring influence on the hardening of polycrystals. In this study, we extend the modeling of dislocation junctions from the binary to multi-junctions, and implement this evolution into a self-consistent visco-plastic model. An application of this model for predicting the yield surface and texture evolution of AA5754 during uniaxial and plane strain loadings is given as a demonstration of the capabilities of the evolutionary binary-multi junction approach.

I. Introduction

The movement and accumulation of dislocations are responsible for the plastic deformation of crystalline materials. The way dislocations interact during movement under specific boundary conditions influences the movement/accumulation of dislocations. It was first assumed that numerous dislocation binary junctions formed due to the 1st order interaction of dislocations (i.e., pairwise interactions) are responsible for deformation behavior of materials. The detailed incorporation of dislocation binary junctions into a crystal plasticity-based constitutive model can describe the evolution of texture and plastic anisotropic response reasonably well [1]. However, it still fails to accurately predict the intensity of main texture components and the evolution of the yield surface. Recent findings show that dislocation multi-junctions also exist, are stable at large deformation, and have a non-trivial influence on the plastic deformation response [2, 3]. The descriptive and predictive capabilities of constitutive models should be improved by incorporating dislocation higher-order interactions into constitutive models. In this study, we will implement the evolution of dislocation interaction from the 1st order to higher order interactions, and discuss the effectiveness of this approach on the modeling of texture and plastic anisotropy of AA5754.

II. Dislocation interactions in Face-centered-cubic (FCC) materials

There are twelve $\{111\}<110>$ slip systems for FCC materials. Dislocation interactions between different slip systems form resultant junctions that hinder the movement of dislocations, leading to latent hardening. Beside the self-interactions of dislocations in the same slip system, there are four categories of binary non-coplanar interactions between dislocations moving on different slip systems during plastic deformation. The most frequent interactions are Lomer-Cottrell interactions, which result in the formation of Lomer-Cottrell (LC) sessile junctions [4, 5]. The other dislocation interactions are Hirth (H), glissile (G) and colinear (COL) [6, 7], resulting in H, G, COL binary junctions, respectively. The binary interactions are often found to be prevalent in polycrystals. However, Bulatov *et al.* showed that higher order interactions (e.g. ternary interaction) also exist, resulting in the formation of multi-junctions which are very stable and greatly influence the strain hardening behavior [2]. Similarly, Madec and Kubin also showed that the ternary interactions can take place in FCC materials, but reported that the ternary junctions did not have as much influence on the plastic deformation behavior as they did in body-centered-cubic (BCC) materials [3]. It is interesting to note that a type of higher order dislocation interaction was studied in detail by Carter quite a long time ago [8]. Carter already discussed the interaction between co-planar multiple partial dislocations and an inclined dissociated dislocation (Fig. 1 in [8]). This higher order interaction can change the character and configuration of both junction and junction nodes significantly.

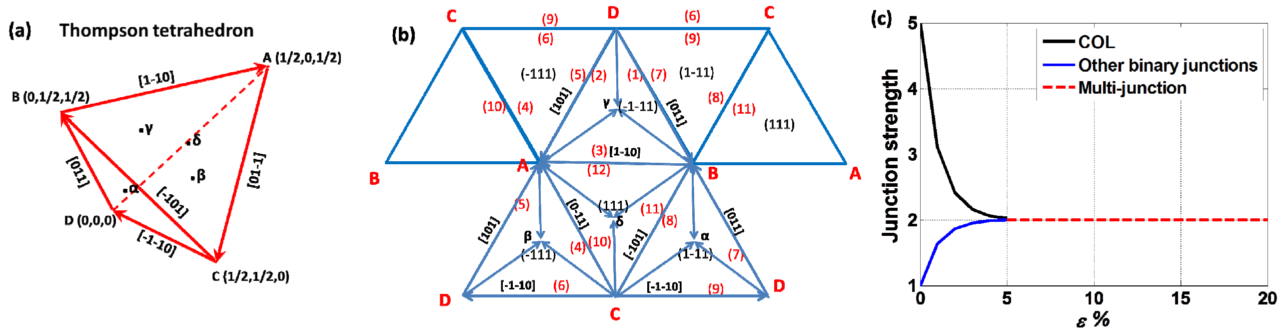

Figure 1: (a) Thompson tetrahedron and (b) its expansion to describe slip systems in FCC materials, (c) The assumed evolution of the strength of dislocation junctions.

Moreover, a recent interesting treatment of dislocation interaction based on the Peierls model by Schoeck showed that there can be a higher-order interaction in a sequential fashion that transforms binary junctions into multi-junctions [9]. For example, a dislocation on slip system 1 interacts with another one on slip system 6 to form a LC lock γβ as follows,

$$\mathrm{BD}, a/2[0\text{-}1\text{-}1] + \mathrm{DC}, a/2[110] = \mathrm{B}\gamma, a/6[1\text{-}2\text{-}1] + \gamma\beta, a/6[10\text{-}1] + \beta\mathrm{C}, a/6[12\text{-}1] \quad (1)$$

Where A, B, C and D are vertices while α, β, γ, and δ are the midpoints of planes of Thompson tetrahedron opposite to A, B, C, and D, respectively (Fig. 1a); and *a* is the lattice parameter.

The LC junction effectively locks other approaching edge dislocations. However, if a screw dislocation on the slip system 5 approaches the LC lock, the stress induced by the stress field of the LC lock on the edge component of the screw dislocation increases. According to Shoeck's treatment, once the imposed stress reaches a critical value, the edge component of the approaching dislocation becomes unstable and collapses [9]. The stopping effect of the LC lock on the screw dislocation no longer holds [9]. A part of the approaching dislocation now can interact with the γβ lock to convert it into a Hirth junction:

$$a/6[10\text{-}1] + a/6[\text{-}10\text{-}1] = a/3[00\text{-}1] \quad (2)$$

The Hirth junction is indeed a multi-junction with two 4-nodes at its ends where three interacting dislocations (on slip systems 1, 6 and 5) and the Hirth junction meet. Schoeck reported that this higher-order interaction would dramatically change the locking effect of the resultant junction since it introduces a screw character into the resultant junction. Along with what was reported in the Carter study [8], not only the character of dislocation junctions, but also the character and configuration of junction nodes are altered after interaction, e.g. expanded nodes can change into contracted nodes. All alternations of junction and nodes influence the locking effect of multi-junctions. The situation becomes complex for super-jogs (i.e. super junctions whose Burgers vector is several times of unit binary junctions), where a junction can partially convert into another type, but its original part is still preserved after interaction.

III. Constitutive equations

At the grain level, the plastic strain rate $\dot{\varepsilon}^p$ is given by the sum of the shear strain rates $\dot{\gamma}^{(i)}$ from all the active slip systems

$$\dot{\varepsilon}^p = \sum_{i=1}^{N} m^{(i)} \dot{\gamma}^{(i)}, \quad (3)$$

where N is the number of slip systems, $m^{(i)}$ is the Schmid tensor of the slip system (i). The Schmid tensor is defined as

$$m^{(i)} = \frac{1}{2}\left(b^{(i)} \otimes n^{(i)} + n^{(i)} \otimes b^{(i)}\right) \tag{4}$$

where b is the slip direction and n is the slip plane normal. The rate at which dislocations move under the influence of a shear stress on their glide plane depends on the magnitude of the shear stress. This rate sensitivity can be modeled as a power-law relationship between the resolved shear stress on slip systems $\tau^{(i)}$ and the shear rate $\dot{\gamma}^{(i)}$ [10],

$$\dot{\gamma}^{(i)} = \dot{\gamma}_0^{(i)} \left|\frac{\tau^{(i)}}{\hat{\tau}^{(i)}}\right|^{1/r} \operatorname{sgn}(\tau^{(i)}) \tag{5}$$

with $\tau^{(i)}$, $\hat{\tau}^{(i)}$ and $\dot{\gamma}_0^{(i)}$ are the Schmid resolved shear stress, the critical resolved shear stress and the reference shear rate for dislocation motion on slip system *(i)*, respectively. Under imposed deviatoric Cauchy stress σ', $\tau^{(i)}$ is given by

$$\tau^{(i)} = m^{(i)} : \sigma', \tag{6}$$

The rate sensitivity r is assumed to be constant during isothermal deformation process and to be equal for all slip systems (r = 20 in this study). The critical stress of the slip system i (i.e., $\hat{\tau}^{(i)}$) evolves during plastic deformation due to the accumulation of dislocation density, which is a function of accumulated plastic strain.

$$\dot{\hat{\tau}}^{(i)} = \frac{d\bar{\hat{\tau}}^{(i)}}{d\gamma} \sum_{i,j,k=1}^{N} h_{ij\times k}\, \dot{\gamma}^{(j)} \qquad (i, j, \text{ and } k = \overline{1, N}\ ) \tag{7}$$

with $\gamma = \sum_{i=1}^{N}\left|\gamma^{(i)}\right|$ and $h_{ij\times k}$ is a hardening matrix induced by dislocation interactions which evolves from binary into higher-order interactions. At the beginning of deformation, a single binary interaction type (e.g., h_{ij}^{COL}) is dominant and governs the material response. During deformation, higher-order interactions (involving the interaction of third dislocations with the existing binary dislocation junctions) occur to transform binary junctions into multi-junctions. This transformation can cause the strength of the initially strongest binary junctions to slightly decrease, while the strength of the new component can gradually increase after interaction. In this study, we first assume that (1) the COL is the strongest binary junction and (2) the strengths of other junctions equals to the strength of self-interaction at the beginning of plastic deformation. The second assumption is that once the multi-junctions form they are stable as reported by Bulatov *et al.*[2]. Stable multi-junctions can undergo a maximum number of three serial higher-order non-coplanar interaction types during deformation. The last assumption is that the strength of a multi-junction does not change if a junction experiences self-interactions or coplanar interactions with other dislocations. This sequential approach to dislocation interactions from first to higher order will cause the strength of dislocation junctions to asymptotically approach the saturation strength of stable multi-junctions. In this study, we assume the saturation strength is the arithmetic mean of the strengths of all four non-coplanar binary junctions. Following the above-mentioned evolution of binary into multi-junctions, the evolution of hardening coefficients can be described by Eq. 8:

$$h_{ij\times k} = \left(h_{ij} - h_{ij\times k}^{sat}\right)\mathrm{e}^{-g\gamma} + h_{ij\times k}^{sat} \tag{8}$$

h_{ij} is the hardening rate associated with binary junctions of slip systems i and j, $h_{ij} = 1$ for $i = j$ and $h_{ij} > 1$ for non-coplanar binary intearctions with $i \neq j$. $h_{ij\times k}$ is the hardening rate associated with $ij \times k$ multi-junctions which are resultants of interaction between the ij binary junction and another dislocation on system k. $h_{ij\times k}^{sat}$ is the average of the strength of all binary junctions involving in the interaction chain. g is a constant to control the degree of deformation where the strength of all multi-junctions converges to $h_{ij\times k}^{sat}$. We set g=100 to let all binary junctions develop into multi-junctions after plastic deformation of about 5 % in this study (Fig. 1c).

IV. Results and Discussions

The AA5754 is weakly textured in the as-received (AR) condition. The initial texture combines recrystallization components (mainly Cube whose intensity was about 4 times random) and some retained rolling components (Brass and Copper orientations) (Fig. 2a). The volume fractions of Brass and Copper components were almost identical, with intensities of about 2 times random [11]. The texture develops fastest during balanced biaxial loading (Fig. 2b) compared to that during other in-plane straining conditions (Fig. 2c, d). The Cube and Copper components are weakened and almost disappear, while the Brass is strengthened after balanced biaxial (BB) strain of 15 % (Fig. 2b).

Table1: Identified parameters for Voce-type law used in [12]

τ_0	τ_1	θ_0	θ_1
37	30	100	33

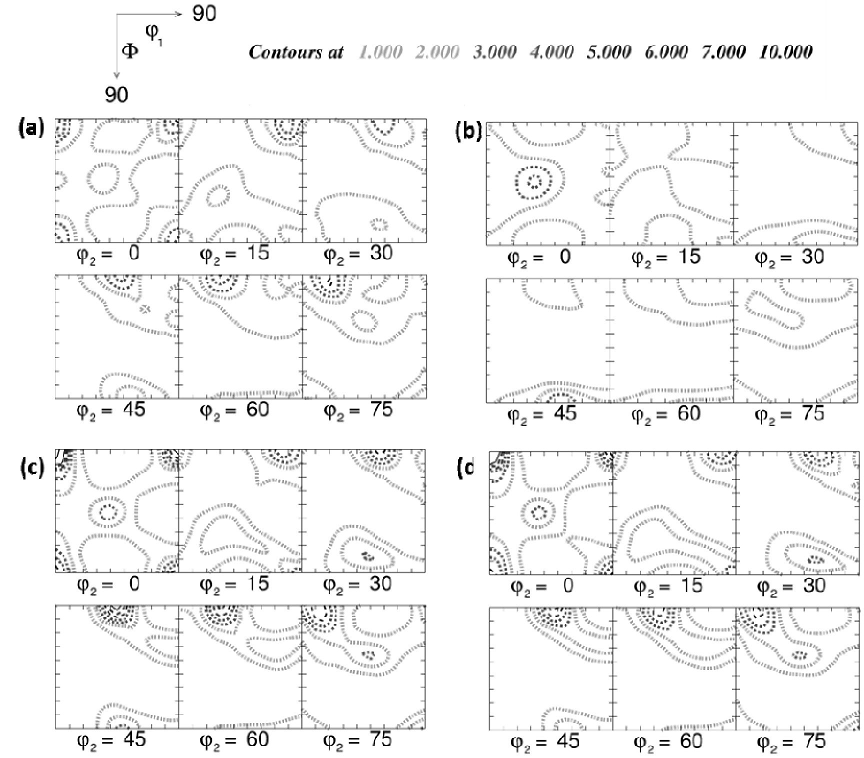

Figure 2: Experimental observation of texture condition (a) of the as-received AA5754 and (b) 15 % balanced biaxial (BB) straining, (c) after 15% unixial straining (U) in rolling direction (RD), (d) 15 % in plane straining (PS) in RD.

Our previous studies showed that crystal plasticity models can predict the evolution of texture, but the models usually over-estimate the intensities even with a very detailed treatment of dislocation binary interaction [1, 13-15]. One possible reason is that the higher order dislocation interactions were neglected in the previous studies. In this study, we assume that at the onset of plastic deformation the COL is the strongest binary junction and equal to 5, while the strengths of other junctions relating to three non-coplanar interaction equal to that of self-hardening. The strengths of COL and other non-coplanar junctions evolve during plastic deformation due to the occurrence of higher order of dislocation interactions as explained in Section II. Finally, all dislocation strengths approach the strength of stable multi-junctions, which is the average of all non-coplanar binary junction types after 5 % (Fig. 1c). This evolution of the strength of dislocation junctions is implemented into visco-plastic self-consistent (VPSC) model [12]. Other parameters relating to the Voce hardening law are the same as used for the binary junction-based VPSC model (Tab. 1). This incorporation of evolutionary dislocation interaction gives a very good prediction of texture intensities after BB of 15 % (Fig. 3a) compared to that by the binary junction based VPSC (Fig. 3b). It also results in a reasonably good prediction of the texture after uniaxial straining and PS parallel to the RD of 15 % (Fig. 3c, d).

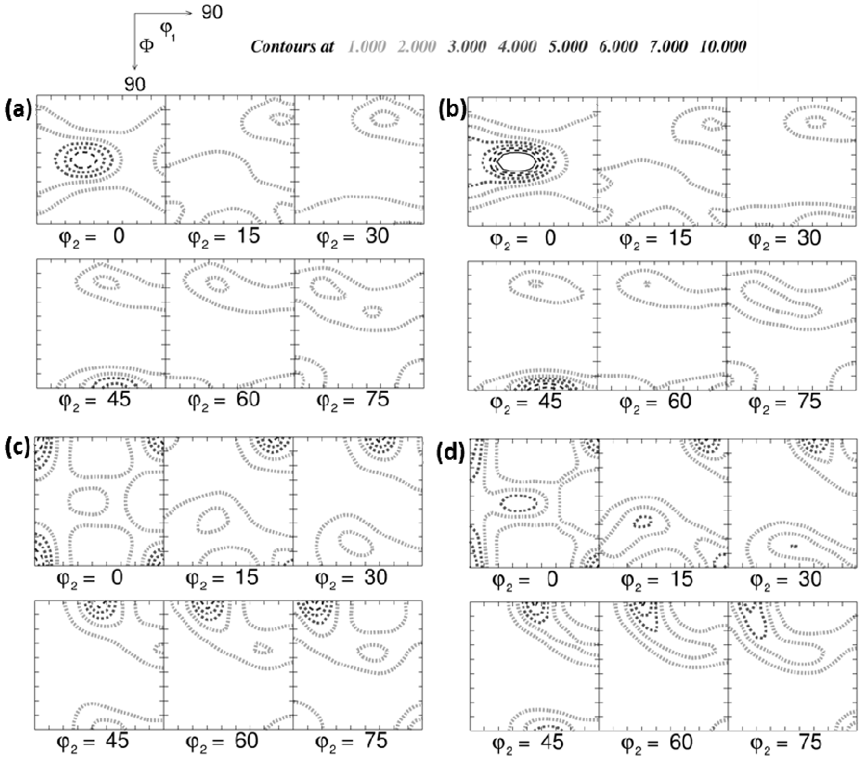

Figure 3: Predictions of texture conditions of 5754 after 15 % of: (a) BB straining by VPSC multi-junction based approach, (b) BB straining by VPSC binary-based approach, (c) U in RD by VPSC multi-junction based approach, (d) PS in the RD by VPSC multi-junction based approach.

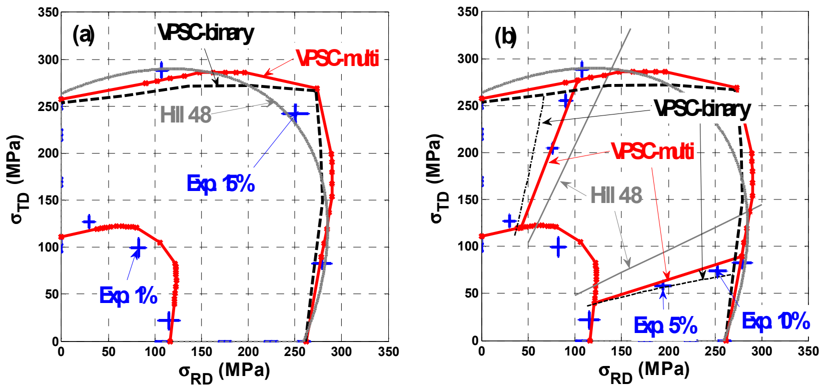

Figure 4: Simulations of (a) yield surface and (b) the stress paths of AA5754 by VPSC and Hill 48 models. Note: The error bars associated with experimental data points in are measurement uncertainties described in Iadicola *et al.* [16].

AA5754 exhibits a complex plastic anisotropy during in-plane straining. The anisotropy is clearly manifested in the evolution of the yield surface as measured and reported in [16]. Compared to the binary junction-based approach, with the same parameters as used for the binary junction-based model (Tab. 1), the multi-junction-based model gives a better prediction of the yield surface after in-plane straining of 15 % albeit it still slightly over-estimates the BB flow stress, and it can not predict well the BB stress path (Fig. 4). Interestingly, the Hill 48 model shows a very good fit regarding the shape of yield surface after 15 % compared to that by VPSC. However, the advantage of the crystal plasticity approach is that it gives a better description of stress paths during in-plane straining, in particular when the uncertainty of controlled strain is taken into account. If we can assume the maximum uncertainty associated with controlled strain in Marciniak plane strain tests is of 10 %, flow stresses corresponding to the strain with an uncertainty of 7.5% being off the nominal value calculated by the multi-junction based VPSC show very good fits for observed stress paths in plane straining compared to those by binary junction based VPSC and by the Hill 48 model with the same uncertainty (Fig. 4b). Together with the improvement of the prediction of the texture development, it corroborates the idea that the multi-junctions not only govern the plastic response of BCC materials but also play a significant role in the response of FCC materials. This finding differs from that of Madec *et al* [3] who suggested that the multi-junctions do not greatly influence the material response. In addition, our recent study [1] shows that by fitting the stress-strain curve using multi-junction based VPSC, the texture development in BB straining can be accurately modeled. An effort is being conducted to see if it also helps to improve the prediction of the yield surface.

Conclusions

The plastic anisotropy of a material can be better modeled by incorporating the higher-order interactions of dislocations into crystal plasticity model compared to a crystal plastic model based on the dislocation first order interactions. In particular, this study shows that the yield surface evolution and texture development of AA5754 during in-plane straining are reasonably well predicted by dislocation multi-junction based model.

References

[1] von Goler F, Sachs G. Tests on crystals of beta measurement. Naturwissenschaften 1928;16:412.
[2] Bulatov VV, Hsiung LL, Tang M, Arsenlis A, Bartelt MC, Cai W, Florando JN, Hiratani M, Rhee M, Hommes G, Pierce TG, de la Rubia TD. Dislocation multi-junctions and strain hardening. Nature 2006;440:1174.
[3] Madec R, Kubin LP. Second-order junctions and strain hardening in bcc and fcc crystals. Scripta Mater 2008;58:767.
[4] Lomer WM. A Dislocation Reaction in the Face-Centred Cubic Lattice. Philos Mag 1951;42:1327.
[5] Cottrell AH. The Formation of Immobile Dislocations during Slip. Philos Mag 1952;43:645.
[6] Hirth JP. On Dislocation Interactions in Fcc Lattice. Journal of Applied Physics 1961;32:700.
[7] B. Devincre, T. Hoc, Kubin L. Dislocation Mean Free Paths and Strain Hardening of Crystals. Science 2008;320.
[8] Tomé CN. Self-consistent polycrystal models: a directional compliance criterion to describe grain interactions. Model Simul Mater Sc 1999;7:723.
[9] Masima M, Sachs G. Mechanical properties of brass crystals. Z Phys 1928;50:161.
[10] Lebensohn RA, Tomé CN. A Self-Consistent Anisotropic Approach for the Simulation of Plastic-Deformation and Texture Development of Polycrystals - Application to Zirconium Alloys. Acta Metall Mater 1993;41:2611.
[11] Banovic SW, Iadicola MA, Foecke T. Textural development of AA 5754 sheet deformed under in-plane biaxial tension. Metall Mater Trans A 2008;39A:2246.
[12] Tomé CN, Lebensohn RA. Manual for Code: Visco-plastic self-consistent (VPSC), version 7d, 2012.
[13] Hu L, Rollett AD, Iadicola M, Foecke T, Banovic S. Constitutive Relations for AA 5754 Based on Crystal Plasticity. Metall Mater Trans A 2012;43A:854.
[14] Iadicola MA, Hu L, Rollett AD, Foecke T. Crystal plasticity analysis of constitutive behavior of 5754 aluminum sheet deformed along bi-linear strain paths. Int J Solids Struct 2012;49:3507.
[15] Kuntze W, Sachs G. The acknowledgement of the yield stress of steel. Z Ver Dtsch Ing 1928;72:1011.
[16] Iadicola MA, Foecke T, Banovic SW. Experimental observations of evolving yield loci in biaxially strained AA5754-O. Int J Plasticity 2008;24:2084.