

Modelling the stored energy of plastic deformation for individual crystal orientations

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Abstract Recovery and recrystallisation processes in polycrystalline metals are driven by the release of energy stored in defect structures chiefly resulting from dislocation creation, motion and interaction during plastic deformation. Some statistical models of texture change during recrystallisation employ the Taylor factor to quantify the distribution of this stored energy amongst orientations. While the Taylor factor is an instantaneous measure of the plastic power dissipation per orientation for a given strain mode, it is technically only valid as an estimate of stored energy if strain path and texture can be assumed constant. This motivates the search for alternatives to the Taylor factor which do not neglect the effects of changing strain path and evolving texture. In this paper a first step is made toward this goal by comparing the Taylor factor with a possible alternative, the accumulated slip per orientation, for a plane strain compression deformation of a bcc material. It is discovered that even for this idealised deformation there are specific orientations for which there is a consistent difference between the two parameters at various magnitudes of strain. It is concluded that these results lend support to the case for replacing the Taylor factor with a history based parameter in recrystallisation texture models.

Introduction

Recovery and recrystallisation processes in polycrystalline metals are driven by the release of energy stored in defect structures chiefly resulting from dislocation creation, motion and interaction during plastic deformation. One approach to modelling the change in texture occurring during discontinuous recrystallisation is to consider the classical nucleation and growth processes as independent orientation selection mechanisms which each permit certain orientations to be present in the final recrystallised texture. In a recent example of such a model [1] nucleation is implemented as a process which selects orientations from the deformation texture on the basis that only those orientations which have both a large volume fraction in the deformation texture and a particular level of stored energy (relative to other orientations) may persist in the recrystallised texture. To date the Taylor factor M of grains in the final discrete texture has been used in the nucleation criterion of the above model as the estimate of the distribution of stored energy amongst the orientations. On its own M is an estimate of the dissipated plastic power per orientation at some moment in time, but can be



used as an estimate of the total dissipated plastic work per orientation on the assumption that (i) the deformation is one of constant strain mode, and that (ii) early in the forming process the orientation of the majority of grains have approached stable orientations. In other words due to assumption (i) the Taylor factor of a grain at any moment during the deformation would be a function only of its orientation at that moment, and due to assumption (ii) the orientation would be only slowly changing for most of the deformation process, so that the value of the Taylor factors for discrete grains in the final state would be approximately proportional to the total plastic work dissipated in those grains. Successful results have been obtained with the recrystallisation model for conventional rolling using the Taylor factor, which supports these assumptions at least for this classic process.

At the same time it is not clear what the limitations of the above assumptions really are, and to which extent they would be valid in a more general forming process, e.g. one with a changing strain path. Thus it is desirable to consider an alternative to the Taylor factor which can account in some way for the full history of deformation, without greatly increasing the complexity of the model.

The accumulated slip Γ is a scalar summation of the absolute value of slip activity on all slip systems of a single grain over some given interval of time. If the critical resolved shear stress τ_c is assumed equal on all slip systems, and strain hardening is assumed not to occur, then Γ can be considered an estimate of the distribution of plastic work amongst orientations and is a possible substitute for M in the recrystallisation model. This paper presents a comparison of M and Γ as estimates of the distribution of stored energy amongst orientations for a monotonic plane strain compression applied to a bcc material.

Computational Method

For a given orientation g both M_g and Γ_g can be calculated for a given macroscopic deformation history, starting from an annealed condition (state of zero stored energy), using the classic full constraints Taylor theory. In this case it is possible to calculate both M_g and Γ_g independently for any orientation g of interest as no grain interaction effects are considered. Furthermore the absolute values of M_g and Γ_g are not of interest, as only the relative values amongst orientations are necessary for the recrystallisation model. This means that for the purpose of the recrystallisation model M_g and Γ_g can be normalised as \tilde{M}_g and $\tilde{\Gamma}_g$ per eqn. 1 without concern for units. In eqn. 1 $\min(A)$ and $\max(A)$ stand respectively for the minimum and maximum of the values of the generic parameter A for all orientations g under consideration.

$$\tilde{A}_g = \frac{A_g - \min(A)}{\max(A) - \min(A)} \quad (1)$$

In this analysis \tilde{M}_g and $\tilde{\Gamma}_g$ are compared numerically in the range (0,1) by contour mapping their values on a $\varphi_2 = 45^\circ$ section in Euler space (Bunge convention). The difference between the two parameters is additionally expressed as a percentage per eqn. 2.

$$\text{rel\%} = \frac{\tilde{\Gamma}_g \times 100}{\tilde{M}_g} \quad (2)$$

Mapping \tilde{M}_g values is straightforward as for a given strain mode they can be calculated directly for any orientation desired. However to obtain corresponding $\tilde{\Gamma}_g$ values the crystal plasticity calculations must be such that, after the desired strain history, a sufficient quantity of grains have a final orientation which happens to fall on the $\varphi_2 = 45^\circ$ plane at the strain of interest. Moreover, there can be a limit to the magnitude of strain that can be applied as the discrete orientations tend to cluster around stable orientations.

Considering the above the following method was employed to calculate contour maps: a full constraints Taylor simulation of plane strain compression was conducted starting with an

initial grid of 891,000 orientations ($0^\circ \leq \varphi_1, \Phi \leq 90^\circ, -10^\circ \leq \varphi_2 \leq 100^\circ$, with 1° spacing); $\{110\}\langle 111 \rangle$ and $\{112\}\langle 111 \rangle$ slip systems were active, with equal critical resolved shear stresses and no strain hardening. A map of \tilde{f}_g values on the $\varphi_2 = 45^\circ$ plane was produced by selecting those grains whose orientations were found to be within in the range $44^\circ \leq \varphi_2 \leq 46^\circ$ at the macroscopic strain of interest. The values of \tilde{f}_g for these grains were extracted and interpolated on to a regular grid to allow generation of contours.

In this analysis the strain mode is constant, thus \tilde{M}_g is constant and the contour map of \tilde{M} for the $\varphi_2 = 45^\circ$ section of Euler space does not change, and need only be calculated once. However in practise the same process was used to calculate both \tilde{f}_g and \tilde{M}_g at every step of the simulation, as a control on the quality of the interpolation, i.e. changes observed in the Taylor factor maps with increasing strain would indicate some numerical error to be present.

Results

Figure 1 (i) and (ii) show the normalised Taylor factor map at a von Mises equivalent strain of 5.7% and 57% respectively: only very small variations are visible, suggesting interpolation error at the largest strain considered to be low. Figure 1 (iii) shows a contour plot of normalised accumulated slip values \tilde{f}_g at a von Mises strain of 57%: the main differences with the corresponding Taylor factors \tilde{M}_g are local to $(\varphi_1 = 90^\circ, \Phi = 10^\circ)$ where $\tilde{f}_g \gg \tilde{M}_g$, and local to $(\varphi_1 = 90^\circ, \Phi = 75^\circ)$, where $\tilde{f}_g \ll \tilde{M}_g$.

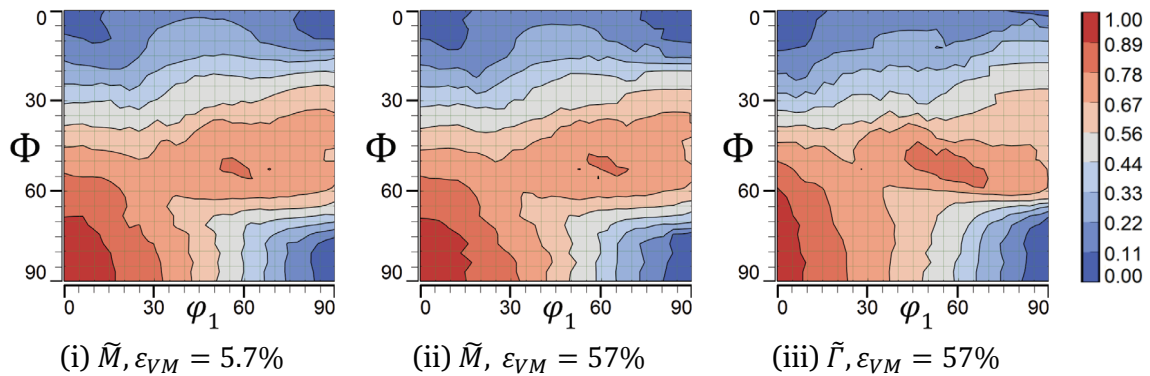


Figure 1. Normalised Taylor factor and normalised accumulated slip maps plotted for $\varphi_2 = 45^\circ$ sections of Euler space for plane strain compression of bcc material: (i) and (ii) show normalised Taylor factor \tilde{M} for von Mises equivalent strain ε_{VM} of 5.7% and 57% respectively; (iii) shows normalised accumulated slip \tilde{f} at 57% ε_{VM} . All values are normalised per eqn. 1.

Figure 2 compares \tilde{M}_g and \tilde{f}_g using the relative values of eqn. 2. The red colour indicates regions where $\tilde{f}_g \gg \tilde{M}_g$, and blues indicates regions where $\tilde{f}_g \ll \tilde{M}_g$. At low strain ($\varepsilon_{VM} = 5.7\%$) Figure 2 (i) indicates no significant difference between \tilde{M}_g and \tilde{f}_g , though two distinct regions of significant difference begin to appear at 11% ε_{VM} , as visible in Figure 2 (ii): one appears between the orientations $(001)[0\bar{1}0]$ and $(112)[\bar{1}\bar{1}0]$, equivalently $(\varphi_1 = 90^\circ, \Phi = 0^\circ)$ and $(\varphi_1 = 90^\circ, \Phi = 17.6^\circ)$, where $\tilde{f}_g \gg \tilde{M}_g$, and another between $(332)[\bar{1}\bar{1}3]$ and the Goss orientation, equivalently $(\varphi_1 = 90^\circ, \Phi = 64.7^\circ)$ and $(\varphi_1 = 90^\circ, \Phi = 90^\circ)$, where $\tilde{f}_g \ll \tilde{M}_g$. These regions grow in size with increasing strain as visible in Figure (iii) at 57% ε_{VM} .

Discussion

Given the successful predictions of recrystallisation texture model for conventional rolling using the Taylor factor as the estimate of stored energy, it was expected no significant

differences should be found between \tilde{I}_g and \tilde{M}_g for this idealised deformation. For most orientations in the $\varphi_2 = 45^\circ$ section of Euler space the two parameters are within 25% of each other, which suggests Γ should at least provide comparably valid predictions when substituted for M in the recrystallisation model.

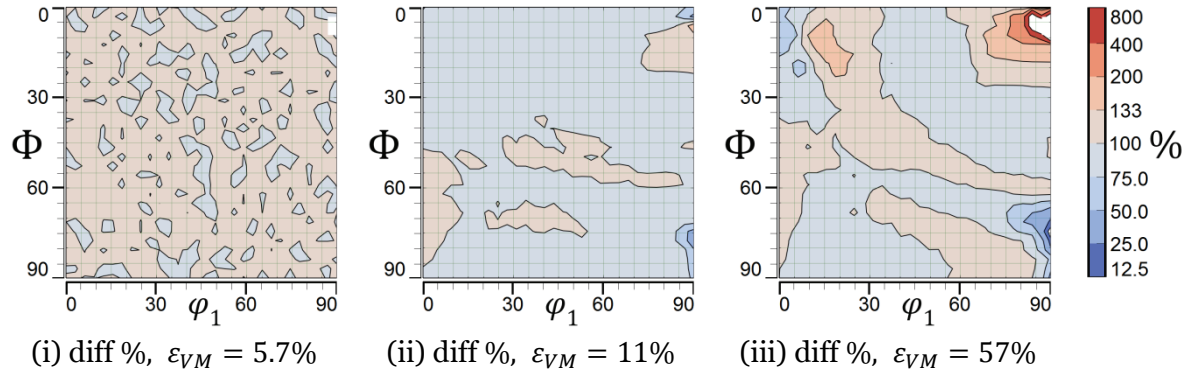


Figure 2. Ratio of accumulated slip divided by normalised Taylor factor per eqn. 2, plotted on $\varphi_2 = 45^\circ$ sections in Euler space for three levels of strain: (i) 5.7%, (ii) 11% and (iii) 57% von Mises equivalent strain ε_{VM} . The white colour indicates regions where $\tilde{I}_g > 800\%$ of \tilde{M}_g .

It is somewhat surprising then to find some specific orientations where the two parameters differ significantly. Both of these regions of difference are close to important texture components in the deformation texture (γ -fibre and (001)[010] component), and notwithstanding other orientation effects (e.g. oriented growth) are thus likely to be significant for the recrystallisation texture.

It is interesting to note that the region where \tilde{I}_g is much lower than \tilde{M}_g , near the (331)[$\bar{1}\bar{1}6$] orientation, coincides with the tendency in some cold rolled steels for orientations in the gamma fibre to shift toward the neighbourhood of the (331)[$\bar{1}\bar{1}6$] orientation [2]. On the other hand, if nucleation in such cold deformed steels is accepted to predominately occur in grains of high stored energy, a direct explanation for this shifting phenomenon would be forthcoming from the current analysis only if \tilde{I}_g were to be higher than \tilde{M}_g , rather than lower as in fact found in these results.

Conclusions

- The normalised accumulated slip predicts a distribution of stored energy amongst orientations largely similar to the normalised Taylor factor for plane strain compression of bcc material.
- There are significant differences observed for the ranges of orientations between (001)[010] and (112)[$\bar{1}\bar{1}0$], and between (332)[$\bar{1}\bar{1}3$] and the Goss orientation.
- There may be some significance to the difference between the two parameters found near the (331)[$\bar{1}\bar{1}6$] orientation: strengthening of the texture near this component has been observed in recrystallisation textures of cold rolled steels.

Acknowledgements

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References

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