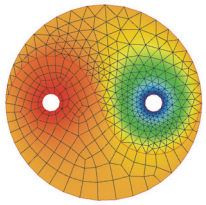
Publishing House
AKAPIT

COMPUTER METHODS IN MATERIALS SCIENCE

Informatyka w Technologii Materiałów

Vol. 7, 2007, No. 1



MODELING OF HOT ROLLING 6061 ALUMINUM ALLOY – STATE VARIABLES AND GRAIN SIZE PREDICTIONS

LUIGI DE PARI JR., ALEXANDER R. BANDAR, WILLIAM H. VAN GEERTRUYDEN, WOJCIECH Z. MISIOLEK

Institute For Metal Forming, Lehigh University
Bethlehem, PA, USA

Abstract

Numerical modeling of hot rolling 6061 aluminum alloy was performed in order to predict state variables: temperature, strain, strain rate, and stress. This was achieved with the finite element modeling package DEFORM 2-D. The state variables were used in a dynamic recrystallization (DRX) model that incorporates both continuous dynamic recrystallization (CDRX) and geometric dynamic recrystallization (GDRX) to predict grain structure evolution. The performed simulation was verified by experimental torsion tests and roll tests from literature. The objective of the present work is to link state variables with the prediction of grain structure evolution.

Key words: continuous dynamic recrystallization, geometric dynamic recrystallization, numerical and physical modeling, 6061 aluminum alloy, grain size, state variables, rolling

1. INTRODUCTION

Numerical modeling provides a useful tool in predicting final material quality in the form of microstructure in place of experimental trial and error. However, current numerical models are not capable of fully predicting the microstructure response reliably. The rolled surface has been especially difficult to predict in terms of microstructure evolution.

The research focus is to understand the grain size evolution of the rolled surface using a dynamic recrystallization (DRX) model that incorporates both continuous dynamic recrystallization (CDRX) and geometric dynamic recrystallization (GDRX). Other attempts to unify microstructure evolution mechanisms have been developed, (Humphreys, 1997a; Humphreys, 1997b; Humphreys & Hatherly, 2004; Nes & Marthinsen, 2002; Pettersen et al., 2003; Suni et al., 2002) however, the lack of easily applicable quantitative models to predict both GDRX and CDRX has been a difficulty. (Bandar, 2005) In addition, current models have underestimated high-angle grain boundary (HAB) development. (Bandar, 2005; Blum et al., 1996; Gourdet et al., 1996; Humphreys & Hatherly, 2004; Pettersen et al., 2003)

As a result of the current state of literature, Bandar (2005) proposed that if both CDRX and GDRX were modeled simultaneously a more realistic model may be achieved to predict experimental observations, including the area of HABs. A new GDRX model was also developed based on a 14-sided three-dimensional space-filling shape known as a truncated octahedron (TO). It was successful in accounting for some of the "missing" HABs. In the current research this joint DRX model is refined and applied to AA6061 hot rolling.

ISSN 1641-8581

2. PROCEDURE - DESCRIPTION OF THE MODEL

Part I. Continuous dynamic recrystallization (CDRX) model

The CDRX model (Gourdet & Montheillet, 2003) employed in this dual evolution model takes into account three mechanisms; strain hardening, dynamic recovery, and HAB migration. They are accounted for by the modified Laasraoui-Jonas equation (Gourdet & Montheillet, 2003), which calculates the change in the internal dislocation density, $d\rho_i$.

$$d\rho_i = (h - r\rho_i)d\varepsilon - \rho_i dV \quad (\mu m^{-2}) \qquad (1)$$

where h (μm^{-2}) and r *(unitless)* respectively represent the strain hardening and dynamic recovery, and the dV term represents the volume swept by the mobile boundaries. Refer to Gourdet and Montheillet (2003) for further details on the CDRX model and material constants. Note, in this work an activation energy, Q, of 156 kJ/mol was used. (Van Geertruyden et al. 2006)

Part II. Geometric dynamic recrystallization (GDRX) model

Contrary to the simplistic cubic representation in previous models, a 14-sided three-dimensional space-filling shape called a truncated octahedron (TO) is used (figure 1a) (Bandar, 2005). This shape is comprised of 8 hexagons and 6 squares, and is nearly equiaxial, which very closely resembles actual grain morphologies within a homogenized polycrystal. (Bandar, 2005; Humphreys & Hatherly, 2004)

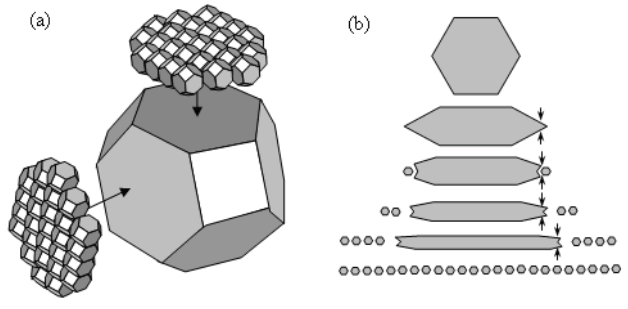


Fig. 1. *Truncated octahedron (TO). (a) Depiction of original grain serration due to the close-packing of subgrains (b) Illustration of geometric dynamic recrystallization (GDRX). (Bandar, 2005).*

Assuming a grain is modeled as a TO with a constant collection of subgrains also modeled as equal sized TOs, it is now possible to determine an analytical relationship between strain and GDRX subgrain break-out. (Bandar, 2005)

First, the total surface area per unit volume of all the boundaries is given by equation (2):

$$S_{Total} = \frac{n_{sg} S_{sg}}{2} \quad (\mu m^{-1}) \qquad (2)$$

where: n_{sg}: number of subgrains within the grain, S_{sg}: area of a single subgrain per unit volume (μm^{-1})

Note; the right-side term is divided by two because each face is shared with its neighbor. The HABs are the large faces of the TO and the low-angle grain boundaries (LABs) are represented by the faces of internal TOs.

The fraction of HABs can be defined as:

$$f_{HAB} = \frac{S_{HAB}}{S_{Total}} \qquad (3)$$

where: S_{HAB}: area of a single grain per unit volume, S_{Total}: total surface area of all the boundaries per unit volume

The fraction of LABs is the balance of f_{HAB} from unity:

$$f_{LAB} = 1 - f_{HAB} \qquad (4)$$

When the grain deforms, its surface area increases while its volume remains constant. This results in an increase for HABs without an increase in the total boundary surface area. (Bandar, 2005)

The average TO diameter can be calculated by proportionally weighing each diameter as shown in equation 5. This is determined by taking the average of the 7 diameters in the TO – the distances between the 4 pairs of hexagonal faces and the 3 pairs of square faces, where each hexagon and square has a leg-length of 'a'.

$$D_{TO} = \frac{\left(4(a\sqrt{6}) + 3(2a\sqrt{2})\right)}{7} = 2.6119a \quad (\mu m) \qquad (5)$$

The volume of a TO is:

$$V_{TO} = 8\sqrt{2}a^3 \quad (\mu m^3) \qquad (6)$$

The relationship between the critical GDRX strain and the TO fraction within this critical region is performed by a Matlab program that models the TO shape change, "geometric shape change" (GSC), as it is stretched (figure 2).

True strain is used for this model:

$$\varepsilon = \ln\left(\frac{l_f}{l_0}\right) \qquad (7)$$

where: l_f: final length of the deformed TO, l_0: initial length of the undeformed TO

As the strain in the Z direction increases or decreases, the strain in the X and Y directions changes

proportionally, according to the TO geometry, to maintain constant volume. (Bandar, 2005)

$$\varepsilon = \ln\left(\frac{Z}{D_{T0}}\right) \tag{8}$$

This allows the modeling of both GSC and GDRX separately; instead of the usual single grouping that other researchers have considered (Nes et al., 2001; Gourdet & Montheillet, 2003; Humphreys & Hatherly, 2004). As the grain changes shape its surface area increases, resulting in a smooth change in the proportion of HABs to LABs. (Bandar, 2005).

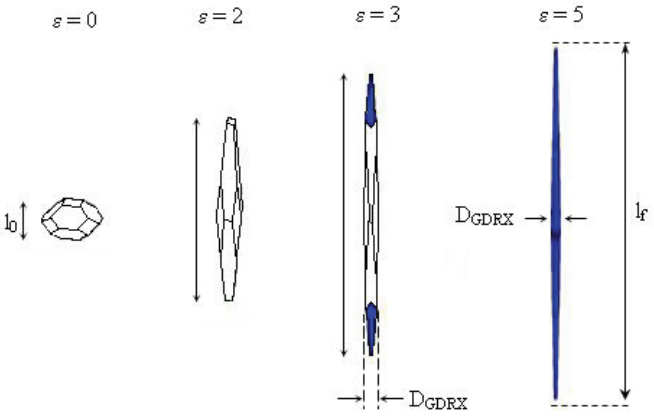


Fig. 2. *The shape of a TO as it appears deformed in tension. The light area indicates regions of the TO which are still wider than the critical strain for GDRX. The dark area indicates regions of the TO which are within the critical condition for GDRX. (Bandar, 2005)*

Joint dynamic recrystallization model: Combined CDRX and GDRX model

In figure 3, Bandar (2005) illustrates the combined CDRX and GDRX mechanism. As deformation begins LABs develop by dislocation accumulation. As strain increases, LABs convert to HABs as the grain begins to thin below the critical GDRX thickness and pinch-off in new 'subgrain-sized' grains due to the serrations from neighboring grains coming into contact (figure 1b).

Quantitatively, the area of HABs per unit volume, S_{HAB}, equals the initial $S_{HAB,i}$, plus HABs due to CDRX, $S_{HAB,CDRX}$, plus any LABS converted to HABs via GSC, $S_{HAB,GSC}$, and GDRX, $S_{HAB,GDRX}$, minus any HABs lost to due to HAB migration (Gourdet & Montheillet, 2003).

$$S_{HAB} = S_{HAB,i} + S_{HAB,CDRX} + S_{HAB,GSC} + S_{HAB,GDRX} - SdV \quad (\mu m^{-1}) \tag{9}$$

The area of LABs per unit volume, S_{LAB}, equals the LABs due to CDRX minus the LABs lost to GSC and GDRX.

$$S_{LAB} = S_{LAB,CDRX} - S_{LAB,GSC} - S_{LAB,GDRX} \quad (\mu m^{-1}) \tag{10}$$

The total surface area per unit volume, S, of all the boundaries is the sum of S_{HAB} and S_{LAB}. (Gourdet & Montheillet, 2003)

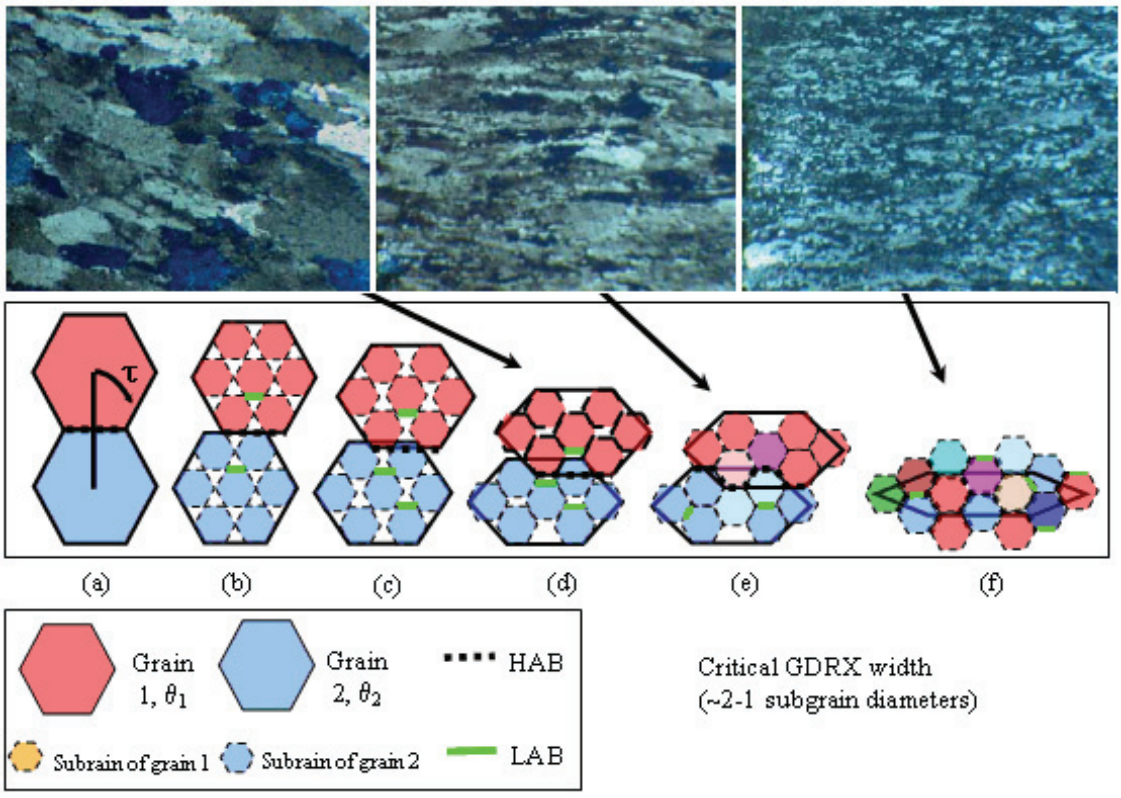


Fig. 3. *TO model illustrating the combined CDRX and GDRX mechanism. (Bandar, 2005) LOM - Van Geertruyden et al., (2006).*

$$S = S_{HAB} + S_{LAB} \quad (\mu m^{-1}) \qquad (11)$$

Simulating hot rolling AA6061: DEFORM 2-D & Joint DRX Model

Applying this model to AA6061 hot rolling involved simulating the rolling process in the finite element modeling package DEFORM 2-D. The initial conditions for the rolling simulation as well as the experimentally rolled samples are displayed in table 1 (Hurley, 2005):

Table 1. *Initial conditions for DEFORM 2-D AA6061 hot rolling simulation*

Material (Slab) Thickness	10.16 mm (0.4 in)
Material (Slab) Temperature	398.88 °C (750 °F),
Roll Diameter	149.22 mm (5.875 in)
Roll Temperature	82.2 °C (180 °F)
Roll Tangential Speed	12.192 m/min (40 ft/min)
75 % Reduction (Single Pass) →	2.54 mm (0.1 in)
Shear Friction Coefficient	0.5
Time Step	0.0025 sec
Mesh Elements	8000

3. RESULTS/DISCUSSION

Initial verification for the accuracy of the model was achieved by comparison to experimental results from literature. Van Geertruyden et al. (2006) presented hot torsion results for AA6061 low-Cr with the following experimental conditions: T = 400˚C, strain = 3.5, and strain rate = 15 s^{-1}. The initial average grain size equaled 124 μm, the resulting average grain size, D_f, equaled 3.78 μm and the fraction of LABs, f_{LAB} equaled 0.77 (figure 4a). Additional parameters set for the joint DRX model were; strain increment, $d\varepsilon$ = 0.030, misorientation angle increment, $d\delta$ = 0.01435˚ (used to reproduce results in Gourdet and Montheillet (2003) when writing CDRX code), and subgrain size, D_{sg}, equals D_f/1.21 (Bandar (2005) experimentally found for the torsion samples that the critical thickness for GDRX to occur was 1.21D_{sg}).

The joint DRX model simulates the experimental f_{LAB} (figure 4b) and average grain size (figure 5a) within an acceptable range. However, the calculated flow curve under-predicts the experimental curve (figure 5b).

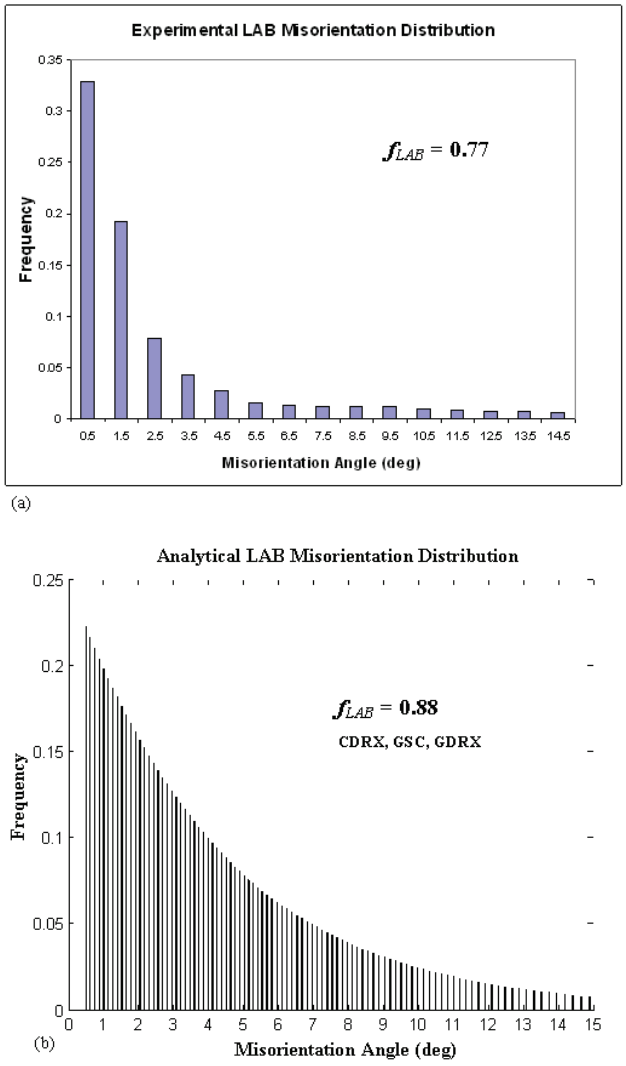


Fig. 4. *(a) experimental and (b) joint DRX model results for LAB misorientation angle after a strain of 3.5.*

For the AA6061 hot rolled simulation, the average initial grain size for the experimental material was 99.8 μm. (Hurley, 2005) The final average grain size, D_f, equaled 4 μm (Hurley, 2005) and the subgrain size, D_{sg}, equaled 4/1.21 μm (Bandar, 2005). The state variables obtained from DEFORM 2-D are temperature, strain, strain rate, and stress. From the model, the average grain size (figure 6a) was reasonably simulated. However, the calculated stress at the rolled surface (figure 6b) was under-predicted.

In both Van Geertruyden et al.'s (2006) experimental torsion tests and the AA6061 experimental rolling tests (Hurley, 2005) the joint DRX results are similar. The final average grain diameter for torsion ($D_{Torsion}$ = 7.76 μm, $D_{model/FEM}$ = 5.65 μm) and rolled samples ($D_{Rolling}$ = 4 μm, $D_{model/FEM}$ = 6.38 μm) are within an acceptable range for the model. The fraction of LAB is also within an acceptable range for torsion; $f_{LAB,Torsion}$ = 0.77, $f_{LAB,model/FEM}$ = 0.88.

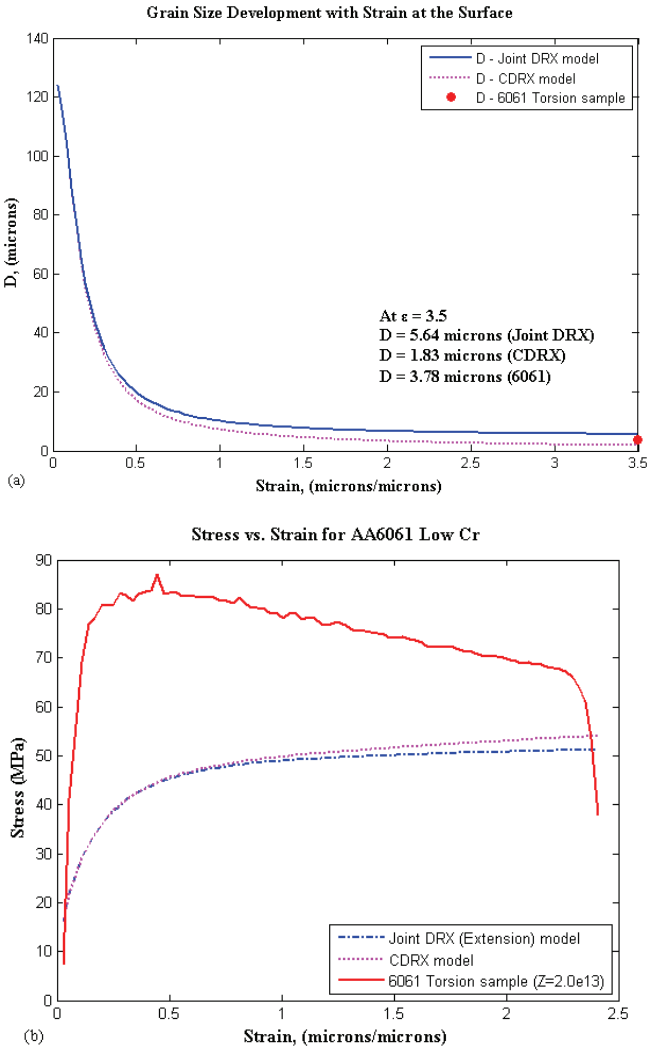


Fig. 5. *Joint DRX and experimental results for (a) average grain size and (b) flow curves.*

However, the joint DRX model needs improvement in simulating the GDRX mechanism. Van Geertruyden et al., (2006) described the microstructure as partially converted to separated subgrains at a strain of 2.5 and fully separated at a strain of 3.5. Yet, GDRX does not begin until a strain of ~6 (figure 7) in the model. This means the calculations are only being influenced by the GSC mechanism and not GDRX. The flow stress inaccuracy may be due to the simple flow stress representation based primarily on dislocation density (Gourdet & Montheillet, 2003). A more accurate model may be Pettersen and Nes's (2003) flow stress model that also accounts for change in texture and the increase in subgrain size during deformation (both of which show evidence for flow stress recovery).

5. CONCLUSIONS

In this study the following conclusions can be made for this modeling effort:

– A joint dynamic recrystallization model incorporating both CDRX and GDRX was created for AA6061 hot rolling.

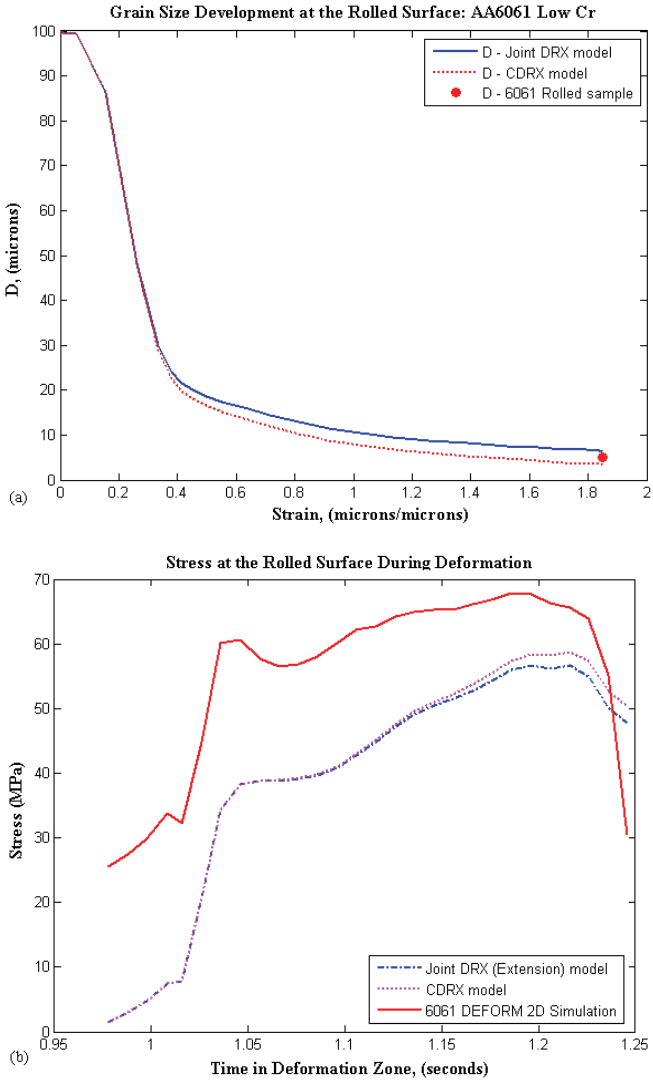


Fig. 6. *Joint DRX and simulated hot rolled results for (a) average grain size and (b) stress at the rolled surface.*

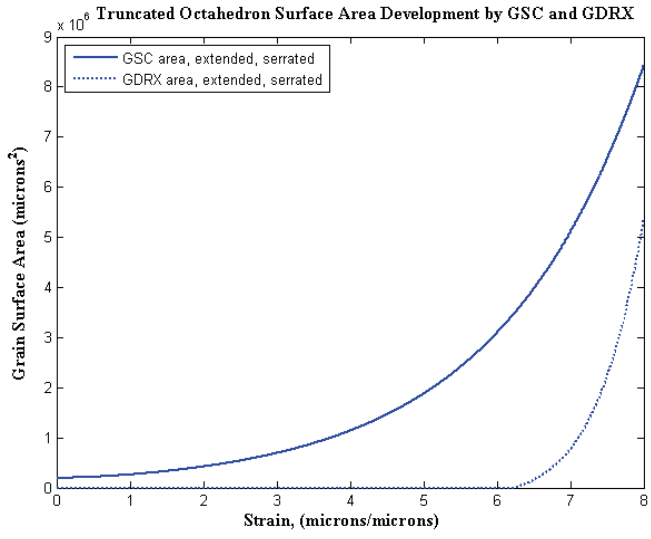


Fig. 7. *TO surface area as a function of strain. D_i = 124 μm, D_f = 3.78 μm.*

- The use of a 14-sided three-dimensional space-filling shape known as a truncated octahedron reasonably simulated the GDRX mechanism as well as successfully accounted for some of the "missing" HABs at the rolled surface.
- Using simulated state variables, the model reasonably predicts grain structure and grain size at the rolled surface.
- The fraction of low-angle grain boundaries and the fraction of high-angle grain boundaries are modeled reasonably well for low strains at the rolled surface.

Theoretical development is still needed for the joint dynamic recrystallization model but in the current state the results are rather accurate.

Acknowledgements. Partial support for Wojciech Z. Misiolek is provided by the Loewy Family Foundation through the Loewy Professorship at Lehigh University.

REFERENCES

Bandar, A.R., 2005, *Modeling Microstructure Evolution in the Dead-Metal Zone of Indirectly Extruded 6061 Aluminum*, PhD Thesis, Lehigh University, Bethlehem.

Blum, W., Zhu, Q., Merkel, R., McQueen, H.J., 1996, Geometric dynamic recrystallization in hot torsion of Al-5Mg-0.6Mn (AA5083), *Mat. Sci. Eng*. A, 205, 23-30.

Gourdet, S., Montheillet, F., 2003, A model of continuous dynamic recrystallization, *Acta Mat*., 51, 2685-2699.

Humphreys, F., 1997, A unified theory of recovery, recrystallization and grain growth, based on the stability and growth of cellular microstructures – I. The Basic Model, *Acta Mat*., 45, 4231-4240.

Humphreys, F., 1997, A unified theory of recovery, recrystallization and grain growth, based on the stability and growth of cellular microstructures – II. The effect of second-phase particles, *Acta Mat*. 45, 5031-5039.

Humphreys, F., Hatherly, M., 2004, *Recrystallization and Related Annealing Phenomena*, Elsevier Ltd., Oxford.

Hurley, N., 2005, *Microstructural evolution during flash annealing of hot rolled 6061 aluminum alloys*, M.S. Thesis, Lehigh University, Bethlehem.

Nes, E., Marthinsen, K., 2002, Modeling the evolution in microstructure and properties during plastic deformation of f.c.c.-metals and alloys - an approach towards a unified model, *Mat. Sci. Eng*. A, 322, 176-193.

Nes, E., Marthinsen, K., Ronning, B., 2001, Modeling the evolution in microstructure and properties during processing of aluminum alloys, *Mat. Proc. Tech*., 117, 333-340.

Pettersen, T., Holmedal, B., Nes, E., 2003, Microstructure development during hot deformation of aluminum to large strains, *Metall. Mat. Trans. A*, 34A, 2737-2744A.

Pettersen, T., Nes, E., 2003, On the origin of strain softening during deformation of aluminum in torsion to large strains, *Metall. Mat. Trans. A*, 34A, 2727-2736A.

Suni, J., Weiland, H., Shuey, R., 2002, Using evolutionary size distributions to model recrystallization in hot rolled, commercial purity aluminum alloys, *Mat. Sci. For*., 408-412, 359-364.

Van Geertruyden, W., Misiolek, W., Wang, P., 2006, Grain structure evolution in a 6061 aluminum alloy during hot torsion, *Mat. Sci. Eng. A*, 419, 105-114.

MODELOWANIE PROCESU WALCOWANIA NA GORĄCO STOPU ALUMINIUM 6061 – PARAMETRY PROCESU ORAZ PRZEWIDYWANA WIELKOŚCI ZIARNA

Streszczenie

Modelowanie numeryczne procesu walcowania na gorąco stopu aluminium 6061 zostało przeprowadzone w celu wyznaczenia takich parametrów procesu jak temperatura, odkształcenie, prędkość odkształcenia oraz naprężenie. Zostało to osiągnięte przy użyciu programu metody elementów skończonych DEFORM 2-D. Parametry procesu wykorzystane w obliczaniach wyznaczono z uwzględnieniem modelu rekrystalizacji dynamicznej (DRX), który składa się zarówno z ciągłej dynamicznej rekrystalizacji (CDRX) i geometrycznej dynamicznej rekrystalizacji (GDRX) w celu wyliczenia ewolucji mikrostruktury. Wyniki przeprowadzonej symulacji komputerowej zostały zweryfikowane własnymi wynikami doświadczalnymi z próby skręcania i walcowania, które są dostępne w literaturze. Celem prezentowanej pracy jest powiązanie parametrów procesu walcowania z wyznaczeniem ewolucji ziarn mikrostruktury.

Submitted: September 19, 2006
Submitted in a revised form: November 8, 2006
Accepted: November 15, 2006