

Antal Kerpely Doctoral School of Materials Science and Technology



Deformation Field, Texture Evolution, and Grain Refinement in Friction-Assisted Lateral Extrusion Process

Thesis Booklet

By

Ali Amininejad

(M.Sc. in Materials Science and Engineering)

Supervisors

Prof. Laszlo S Toth, D.Sc.

Prof. Valeria Mertinger, D.Sc.

Head of the Doctoral School

Prof. Valeria Mertinger, D.Sc.

Institute of Physical Metallurgy, Metal-forming and Nanotechnology

University of Miskolc

Miskolc, Hungary

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Part 1: Deformation Field and Texture Analysis in FALEP

1.1. Introduction

Over the past decades, severe plastic deformation (SPD) techniques have attracted considerable attention due to their capability to produce bulk ultrafine-grained (UFG) structures by imposing extremely large strains. While conventional metal-forming techniques, such as rolling, forging, and drawing, exhibit technical limitations for large plastic deformation, SPD techniques have been shown to be effective alternatives for this purpose [1, 2]. Numerous studies have demonstrated that UFG microstructures generated by SPD processing lead to significant improvements in the physical, mechanical, and functional properties of materials [3, 4]. Various

SPD techniques have been developed, among which high-pressure torsion (HPT), equal-channel angular pressing (ECAP), and accumulative roll bonding (ARB) are the most widely used.

The friction-assisted lateral extrusion process (FALEP) is a novel SPD technique for producing UFG metal sheets from initial bulk or powder material in one single deformation step at room temperature [5, 6]. FALEP benefits from a unique advantage: an additional moving tool (driving punch) laid horizontally at the bottom of the sample that moves in the same direction as the material flow and assists the extrusion process. Fig. 1 presents a schematic illustration of the FALEP technique. While the normal punch provides compression pressure to maintain a non-sliding condition at the interface between the driving punch and the material, the driving punch itself facilitates the material deformation by applying a friction force. The unique design of FALEP allows imposing extremely large shear strains, exceeding 100, on initial bulk or powder materials to produce UFG sheet products in a single operation step at room temperature, making it a highly promising SPD technique for industrial applications.

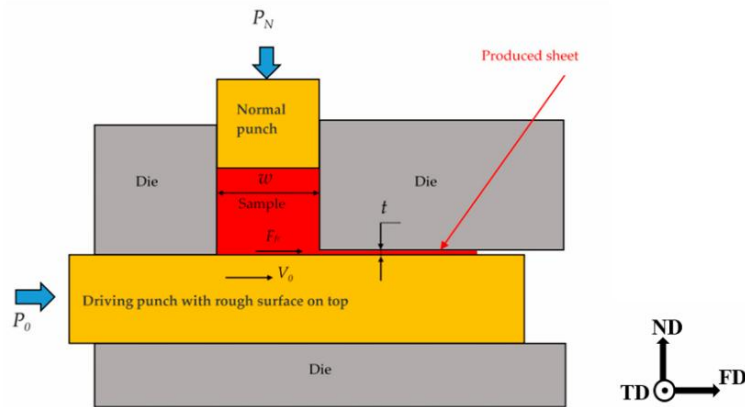


Fig. 1. Schematic of the friction-assisted lateral extrusion process (FALEP) [5].

1.2. Research Questions and Objectives

Due to the novelty of the FALEP technique and the limited number of available studies, several aspects of this processing technique remain poorly understood, particularly the deformation mode and material flow characteristics. Accordingly, the primary objective of the present study is to evaluate deformation behavior during FALEP processing. To this end, a new analytical flow line model is proposed based on experimental observations to describe the deformation mode and to estimate the equivalent strain imposed during FALEP. Using the new flow line model and polycrystal plasticity approaches, texture evolution during FALEP processing is simulated. The proposed model is indirectly validated through quantitative comparisons

between the measured and simulated textures. In the following sections, the experimental procedures and results, the principles of the new modelling approach, and the texture simulation outcomes are presented and discussed in detail. Overall, this study aims to answer the following research questions:

1. What is the deformation mode during the FALEP process at intermediate extrusion ratios?
2. What is the interplay between the imposed deformation and the microstructure and texture evolution in the FALEP process?
3. What is the effect of extrusion ratio on the deformation uniformity across the sheet thickness?
4. Can the classic simple shear model accurately describe deformation and predict texture evolution for intermediate extrusion ratios in the FALEP process?
5. What modeling approaches can be employed to describe the deformation mode and material flow in the FALEP process?
6. What is the role of microstructure evolution and grain refinement in the capability of different polycrystal plasticity models for predicting texture evolution?

1.3. Experimental Procedures and Results

1.3.1. Flow Line Experiments

FALEP experiments were carried out on commercially pure Al-1050 alloy at room temperature using the FALEP facility at the LEM3 laboratory (Metz, France). In total, nine FALEP experiments were performed with a constant ingoing channel cross-section of $20 \times 20 \text{ mm}^2$. The exit channel size, however, varied between 4.3 and 1.1 mm, corresponds to extrusion ratios p/c ranging from 4.6 to 18. In all experiments, the normal punch applied a constant pressure of $P_{ND} = 160 \text{ MPa}$ (6.4 tons), while the driving punch was operated at a constant displacement rate of 3 mm/s. To directly investigate the material flow kinematics during FALEP, each sample was split into two identical parts along the middle of their longitudinal axis prior to deformation. Trajectory lines were then engraved longitudinally only on the surface of one part using either laser marking or CNC machining, depending on the specimen. The two parts were inserted into the FALEP die such that the marked surface was positioned at the internal interface between the two parts, thereby the effect of friction between the marked surface and the die surface was avoided. Fig. 2 shows the marked part of all samples after FALEP processing for the different applied extrusion ratios (p/c).

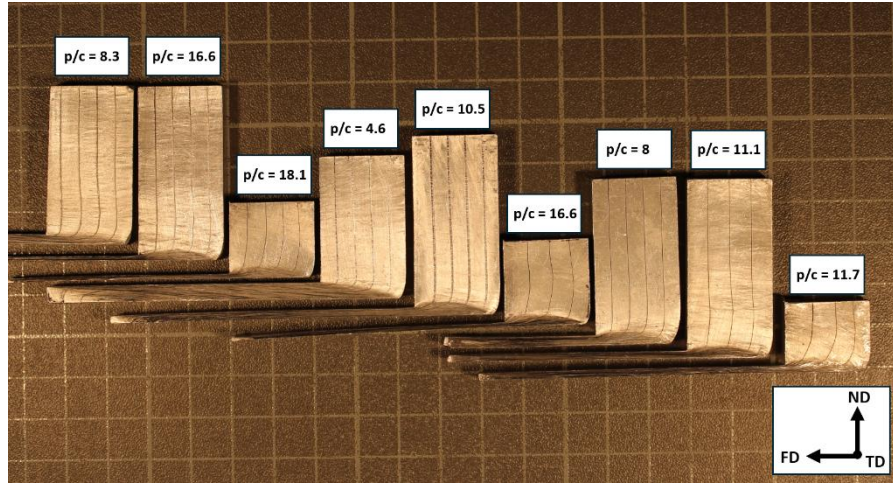


Fig. 2. The marked surface of the samples after FALEP processing at different extrusion ratios (FD = FALEP direction, ND = normal direction, TD = transverse direction).

1.3.2. Microstructure and Texture of Al-FALEP Sample

The microstructure and crystallographic texture of the aluminum sample after FALEP processing at the extrusion ratio of 10.5 were characterized by the EBSD technique using a JEOL JSM-6500F field-emission gun scanning electron microscope. Two regions on the lateral surface of the produced sheet (FD-ND plane) were examined, one located near the top surface (Line1) and the other near the bottom surface (Line4), as shown in Fig. 3. The EBSD data were analyzed using the ATEX software [7]. The initial microstructure and texture of the material were investigated using optical microscopy and XRD (Bruker D8 Advance Diffractometer), respectively. Furthermore, the texture of the bottom surface (Line4) was also measured by XRD on the FD-TD surface to obtain good statistics.

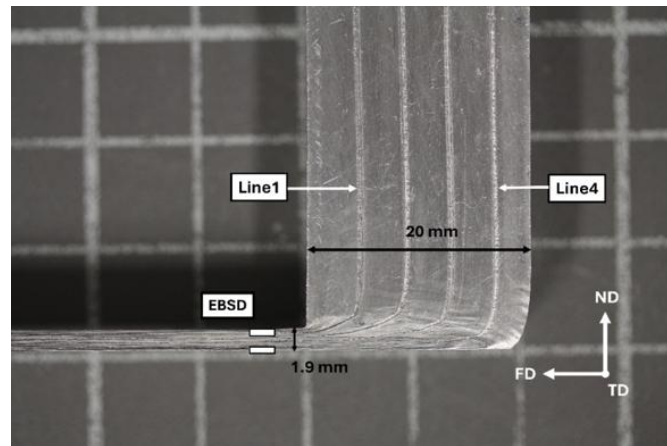


Fig. 3. The marked part of the Al-1050 sample after FALEP processing at an extrusion ratio of 10.5.

The initial microstructure of the Al-1050 sample before the FALEP process is shown in Fig. 4a. The microstructure consisted of coarse grains with an average grain size of approximately 100 μm . During FALEP processing, grain refinement occurred intensively along both the Line1

and Line4 regions. At the end of Line1, a homogeneous and equiaxed grain structure with an average area-weighted grain size of about 720 nm was obtained (Fig. 4b). However, the average grain size at the end of Line4 is significantly larger, reaching approximately 4.2 μm , and the microstructure contains a fraction of relatively coarse grains that are not fully recrystallized, as shown in Fig. 4c. These results clearly indicate the development of a gradient microstructure across the thickness of the produced sheet, with a finer microstructure obtained near the top surface.

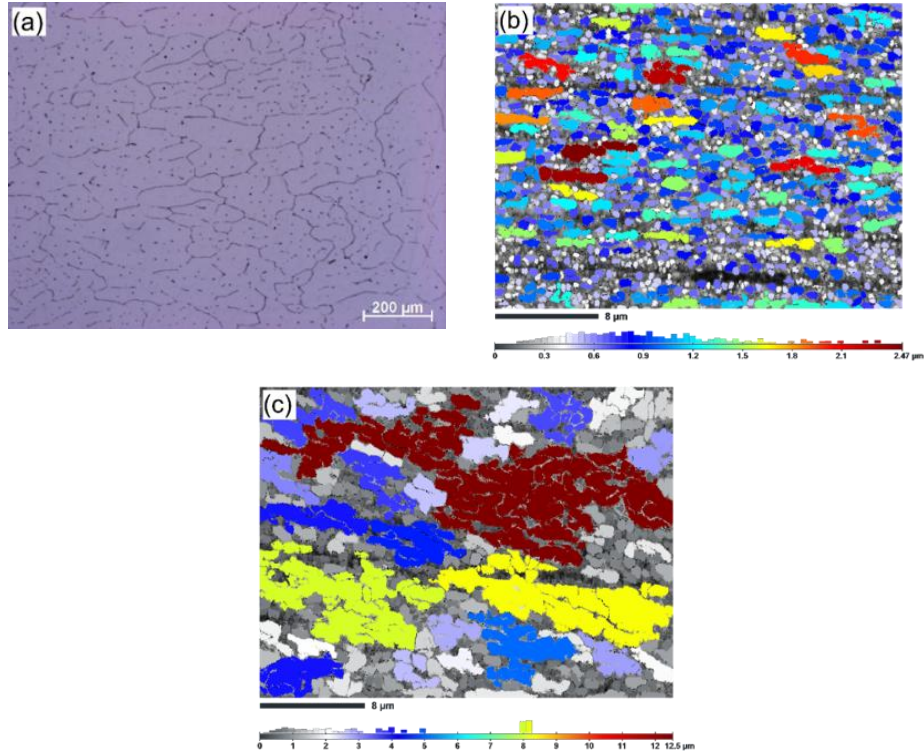


Fig. 4. (a) Optical microscopy image of the initial Al-1050 sample microstructure. SEM micrographs of the sample after the FALEP process (b) near Line1, and (c) near Line4. The grains are colored according to the grain size scale.

1.4. The Three-Stage Flow Line Model

A closer inspection of the trajectory lines reveals that the deformation zone extends significantly above the intersection zone of the two channels, with its upper boundary outlined by the top white broken line in Fig. 5a. Notably, sharp variations are observed in the shape of the flow lines, indicating non-uniform kinematic behavior along the deformation path. Based on these observations, three distinct deformation stages can be identified. In the first stage, the material element undergoes a simple shear deformation before entering the intersection zone, where a pronounced change in flow line direction occurs. Following the first shear deformation, the material element enters a second deformation region in which the trajectory line becomes nearly straight and converging. Finally, a second shear occurs near the exit channel, aligning the line parallel to the exit direction. The relative contribution and sharpness of these three deformation stages become more pronounced by moving from the outer corner (Line4) to the inner corner (Line1). The second stage, referred to here as linear converging extrusion (LCE), has not been reported in previous studies on equal or non-equal channel angular pressing [8, 9]. Nevertheless, this deformation stage can considerably contribute to the total deformation and the resulting texture evolution within the sample. An analytical model is proposed to describe the deformation using the velocity gradient tensor within the LCE zone of the flow

line. For the two simple shear stages, the velocity gradient tensor remains constant and can be directly determined from the orientation of the shear plane. Fig. 5b presents a schematic illustration of the flow lines, highlighting the three deformation stages and their associated geometrical parameters. For the two simple shear stages, the velocity gradient tensor expressed in the laboratory reference system (x-y-z).

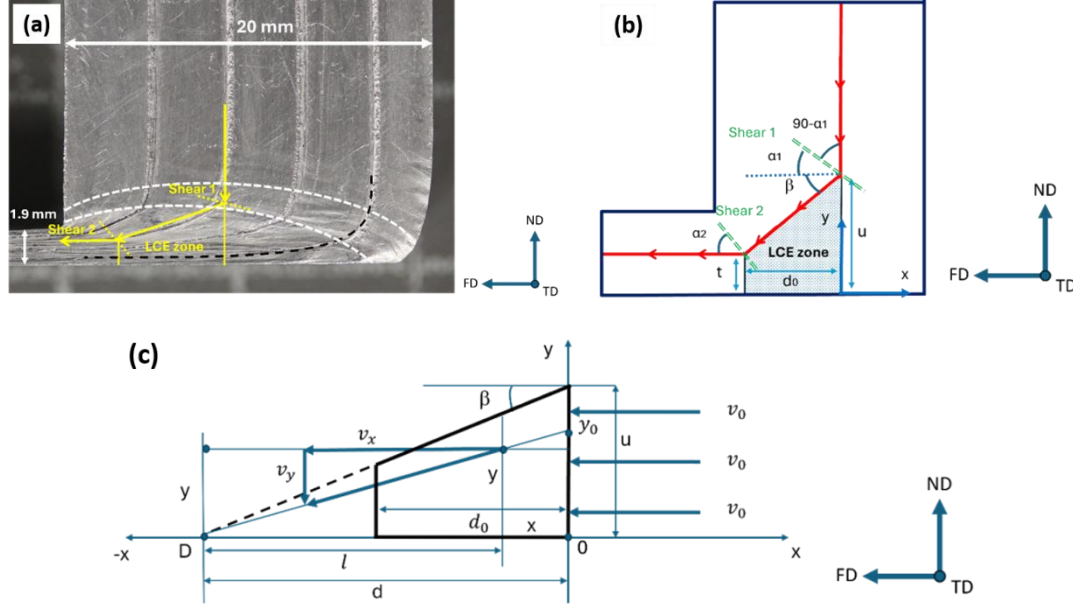


Fig. 5. (a) The three deformation stages along the flow lines (Shear1, linear converging extrusion (LCE) zone, Shear2). (b) Schematic view of the proposed three-stage flow line model for FALEP deformation. (c) Schematic of the LCE zone of the flow line (the thick black lines represent the LCE zone of the deformation field).

Fig. 5c displays a schematic representation of the LCE section of the flow line, in which linear convergent extrusion takes place. In this model, the velocity field is assumed to be radial and directed toward point D . The incoming velocity is denoted by v_0 . The die length is d_0 , while its prolongation projected onto the x-axis is denoted by d . Both quantities are dimensional parameters of the die geometry and therefore take positive values. The flow line function for the LCE part of the deformation is as follows:

$$f(x, y) = \frac{y}{\left(1 + \frac{x}{d}\right)} = y_0 \quad (1)$$

Based on the 2D fluid mechanics, the velocity gradient components of LCE deformation can be calculated. Among them, only three components are non-zero:

$$L_{xx} = \frac{\partial v_x}{\partial x} = \frac{|v_0|}{d \cdot \left(1 + \frac{x}{d}\right)^2} \quad (2a)$$

$$L_{yy} = \frac{\partial v_y}{\partial y} = - \frac{|v_0|}{d \cdot \left(1 + \frac{x}{d}\right)^2} \quad (2b)$$

$$L_{yx} = \frac{\partial v_y}{\partial x} = \frac{2 \cdot |v_0| \cdot y_0}{d^2 \cdot \left(1 + \frac{x}{d}\right)^2} \quad (2c)$$

The selected parameters of the polycrystal plasticity simulations for Line1 and Line4 are summarized in [Table 1](#).

Table 1. Data corresponding to flow lines. Data in italics are parameters of modeling.

	Line1	Line4
Extrusion speed (v_0) mm/s	1	1
<i>LCE zone angle (β)</i>	23°	4°
<i>Length of the LCE deformation zone (d_0) mm</i>	3.5	1
<i>Starting y coordinate on the flow line (u) mm</i>	3.12	0.53
<i>Angle between the first shear plane and the x-axis (α_1)</i>	40°	15°
<i>Angle between the second shear plane and the x-axis (α_2)</i>	15°	90°
First shear value	1.34	3.16
Second shear value	2.45	0.07
Equivalent von Mises strains (shear1, LCE, shear2)	0.78, 0.79, 1.41	1.83, 0.16, 0.04
Total Equivalent von Mises strain	2.98	2.03

1.5. Polycrystal Texture Simulations

Texture simulations were carried out using the viscoplastic self-consistent approach (VPSC, version 5, [10]) in a tuned version, in which a scalar parameter ($1/\alpha$ in the VPSC formulation) was incorporated into the interaction equation of the VPSC model. Several values of the $1/\alpha$ parameter were examined, including the limiting case of $1/\alpha = 0$, which corresponds to the classical Taylor assumption of uniform deformation. For clarity and ease of comparison, this limiting case ($1/\alpha = 0$) is hereafter referred to as the Taylor model. In all simulations, the 12 $\{\bar{1}11\}\langle 110 \rangle$ slip systems were employed with a slip-viscosity exponent of 7 ($1/m = 7$). To assess the effect of the initial texture, two different initial orientation sets were considered: 5000 randomly distributed orientations and 5000 orientations discretized from the experimentally measured initial texture using the ATEX software. The variable velocity gradient derived from the new flow line model was used as input to the polycrystal model to compute the lattice rotations and, consequently, the texture evolution. Meanwhile, texture simulations were also performed using the classical simple shear model for comparison with

the new flow line model. Fig. 6 presents the simulated textures obtained using the classical simple shear model of angular extrusion. The simulations were performed within the Taylor framework, considering both an initially random texture and an initial texture discretized from the experimental measurements. Quantitative comparison with the experimental textures confirms that the agreement between simulation and experiment is poor for both initial random and initial measured textures. Moreover, the simple shear model assumes a uniform shear value and deformation mode along the entire shear plane. As a result, this approach is unable to account for the observed heterogeneity in deformation and texture across the sheet thickness.

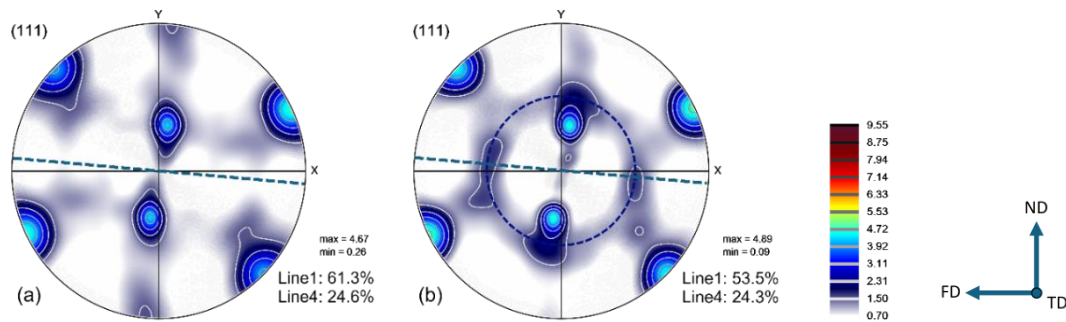


Fig. 6. Pole figures of the simulated textures using the simple shear model for (a) initial random texture and (b) initial measured texture. The correlation indices between simulation and experiment are written next to the pole figures in % for both Line1 and Line 4. The broken line represents the orientation of the intersection plane of the FALEP channels.

Fig. 7 presents the texture simulation results for Line1 using the proposed flow line model, considering three different cases: (i) the Taylor polycrystal model ($1/\alpha = 0$) with an initially random texture, (ii) the Taylor model with the initially measured and discretized texture, (iii) the self-consistent approach with $1/\alpha = 2.5$ using an initial random texture. Interestingly, the best agreement with the experimental texture was achieved using the Taylor model ($1/\alpha = 0$) with the initial random texture (Fig. 7a). In this case, almost all major texture components observed in the measured texture (Fig. 7d) were faithfully reproduced in the simulation. The direct correlation index between simulated and measured texture reached a very high value of 86.3%. Increasing the interaction parameter ($1/\alpha$) from 0 to 2.5 (Fig. 7b), which represents a significant deviation from the Taylor uniform strain assumption, resulting in a reduced correlation index of 55.3%. Fig. 7c displays the simulated texture for Line1 obtained using the Taylor model with the discretized initial texture, rather than a random initial texture. The resulting direct texture correlation index was 77.5%, which is relatively high but is considerably lower than the 86.3% obtained with the initial random texture.

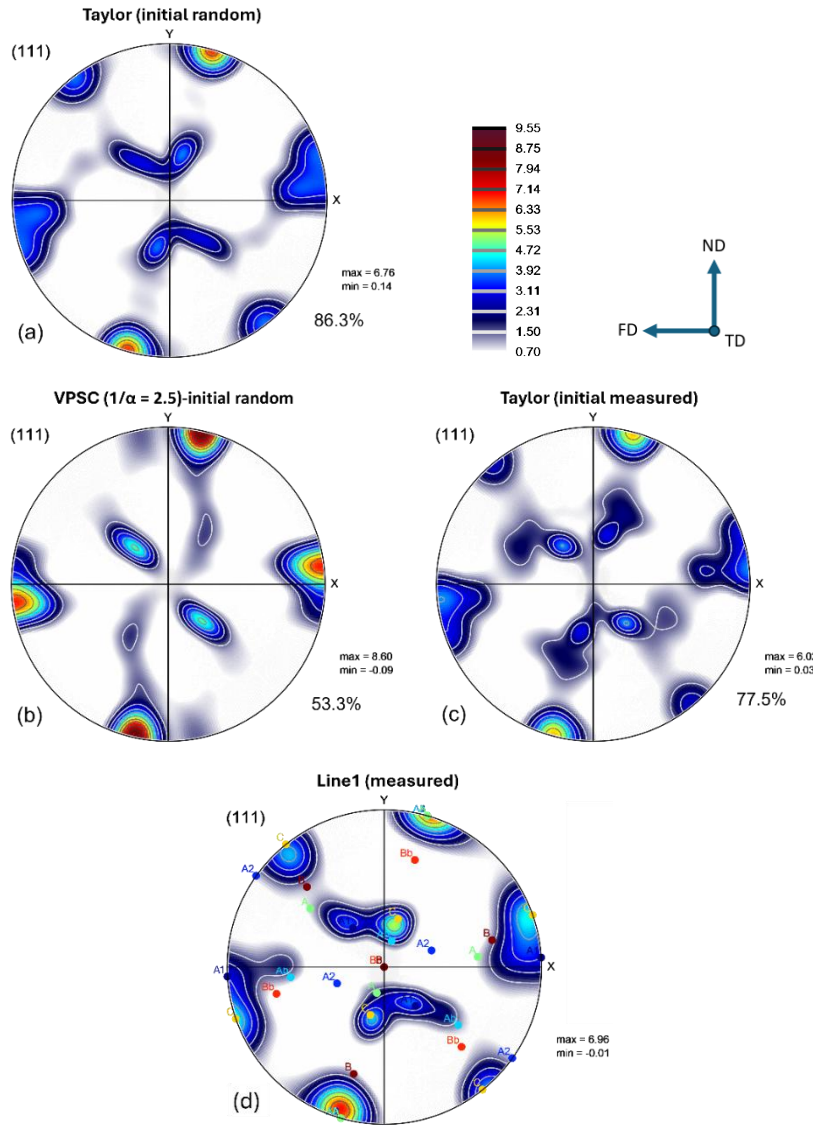


Fig. 7. Pole figures of simulated textures of Line1 using the new flow line model. **(a)** Taylor model with initial random texture. **(b)** Initial random texture with self-consistent model and an interaction parameter of 2.5. **(c)** Taylor model with initial measured texture. **(d)** Experimental texture of Line1.

Fig. 8 shows the texture simulation results for Line4. The highest direct correlation index, 77.3%, was achieved using the self-consistent model with an interaction parameter of $1/\alpha = 7$ and initial orientations discretized from the measured texture. Analysis of the flow line deformation behavior indicates that the three-stage deformation mode was less pronounced for Line4. In particular, the first shear zone was more extended for Line4, during which the flow line became curved and gradually changed its direction. The best agreement between simulated and experimental textures was achieved when the contribution of the LCE stage was relatively small. When the Taylor model with the measured initial texture was employed for Line4, the agreement between the simulated and experimental textures decreased to 67.6% (Fig. 8b). The correlation index was further reduced to 56% when the initial random texture was used with the Taylor model (Fig. 8c).

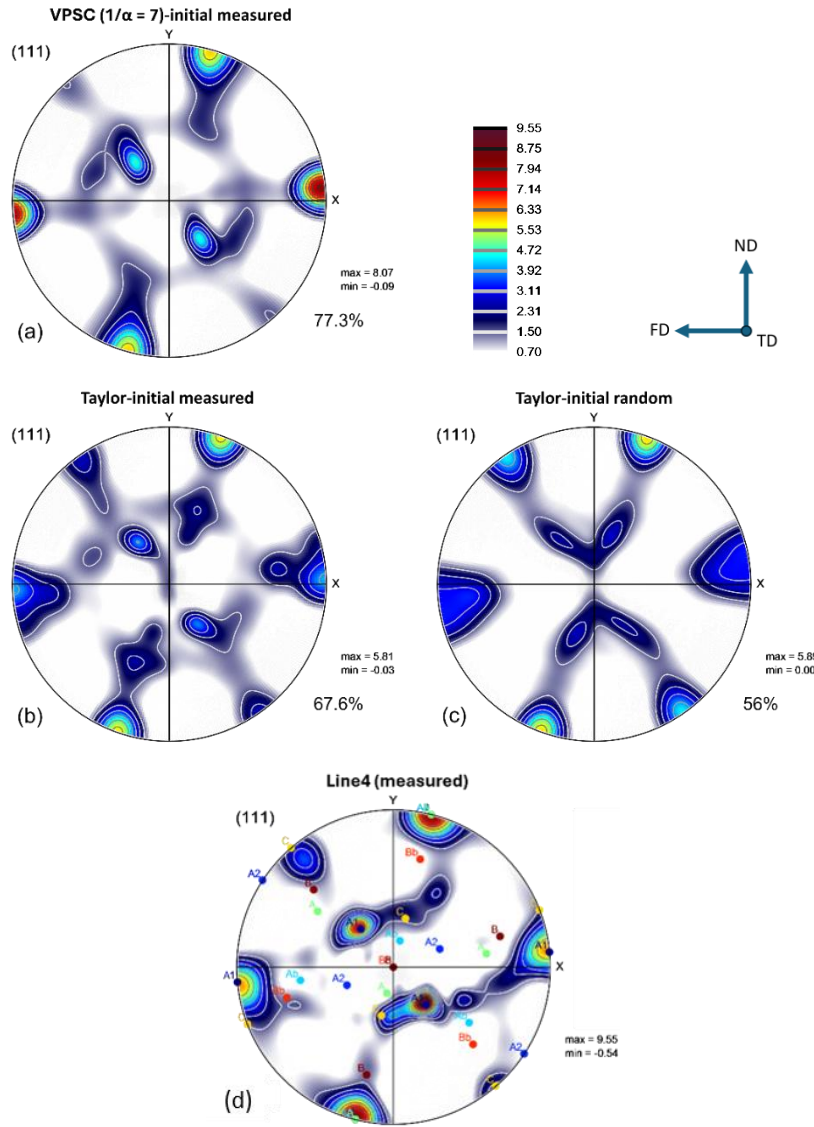


Fig. 8. Pole figures of simulated textures for Line4. **(a)** VPSC model using the initial measured texture with an interaction parameter of 7. **(b)** Taylor model with initial measured texture. **(c)** Taylor model with initial random texture. **(d)** Experimental texture of Line4.

Part 2: Theory of Grain Fragmentation and Grain Coalescence

2.1. Introduction

It is widely accepted that the primary objective of applying SPD techniques is to refine the microstructure down to the ultrafine-grained (UFG) regime, thereby enhancing the material strength through the well-known Hall-Petch law [11, 12]. Therefore, it is essential to explore the mechanisms of grain refinement in plastic deformation. Grain refinement during plastic deformation occurs through dynamic recrystallization (DRX). DRX mechanisms are generally classified into two categories: continuous dynamic recrystallization (CDRX) and discontinuous dynamic recrystallization (DDRX). A schematic representation of these two mechanisms is

shown in Fig. 9. CDRX is the dominant recrystallization mechanism in materials with high stacking fault energy, such as aluminum. During plastic deformation, dislocation annihilation and rearrangement can occur through a recovery process. The rearranged dislocations form dislocation walls with low-angle grain boundaries (LAGBs) within the original grains. The disorientation between subgrains progressively increases during deformation, leading to the transformation of LAGBs into high-angle grain boundaries (HAGBs). Consequently, new grains are formed through the progressive subdivision of the original grains. DDRX, however, is common in low stacking fault energy materials, such as austenitic stainless steels. This mechanism involves the nucleation and growth of small, equiaxed, dislocation-free grains. Therefore, grain boundary migration plays a key role in the DDRX process [13]. In this study, the focus is placed on grain refinement through CDRX, which can be regarded as grain fragmentation. Therefore, the nucleation and growth of new grains associated with DDRX are beyond the scope of this work.

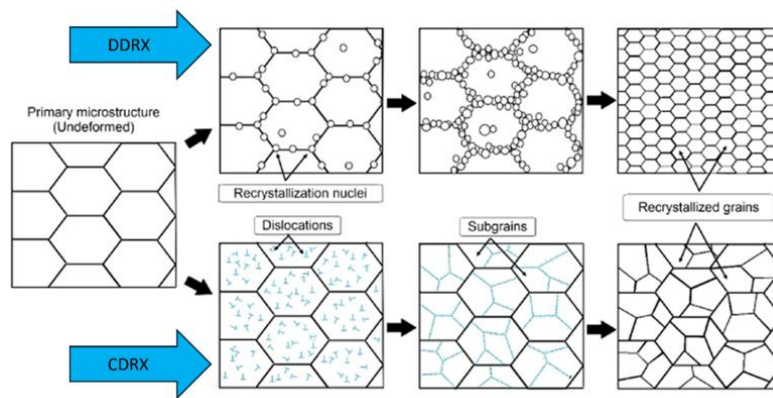


Fig. 9. Schematic illustration of the DDRX and CDRX mechanisms [14].

2.2. Research Questions and Objectives

The primary objective of the second part of this study is to evaluate the role of texture evolution in grain refinement during shear deformation. Based on the experimental observations, the possibility of dynamic grain coalescence induced by texture evolution is examined. An existing grain fragmentation model is optimized to quantify fragmentation and coalescence events during large shear deformation. The aim is to quantitatively analyze grain size evolution under the influence of texture evolution. At the end of this study, the following questions should be answered:

1. What is the role of texture evolution in continuous dynamic recrystallization?
2. Why do the larger grains in the microstructure of the Cu-FALEP sample tend to occupy ideal shear orientations?

3. Is it possible to have grain coalescence at intermediate strain levels before the steady-state grain size? If so, under what conditions?
4. What is the interplay between texture evolution and grain refinement for the rotated-cube fiber?
5. What modeling approach can be used to quantitatively investigate grain fragmentation and coalescence under the influence of texture evolution?

2.3. Experimental Procedures and Results

2.3.1. FALEP of Copper Sample

A commercially pure copper sample was processed via the FALEP technique at room temperature using the FALEP machine at the LEM3 laboratory in Metz. The specimen was a square billet with a cross-section of $20 \times 20 \text{ mm}^2$. The entry and exit channel dimensions of the FALEP die were 20 mm and 2.3 mm, respectively, corresponding to an extrusion ratio of 8.8. Microstructural and crystallographic texture analyses were performed by EBSD using a JEOL JSM-6500F field-emission gun scanning electron microscope. EBSD measurements were conducted on the lateral surface (FD-ND plane), and the data were analyzed using the ATEX software.

2.3.2. Microstructure and Texture of Cu-FALEP Sample

Fig. 10a shows the grain size map which displays a non-uniform distribution, where relatively large grains are embedded within a matrix of well-refined grains. The area-weighted initial average grain size was $35 \text{ }\mu\text{m}$, and the same after FALEP processing was $1.2 \text{ }\mu\text{m}$, confirming that a UFG microstructure was successfully produced. Fig. 10b shows the next-grain-neighbor disorientation distribution of the Cu-FALEP sample. The random Mackenzie distribution is also presented by a solid black line. Notably, the disorientation distribution of the Cu-FALEP sample deviates from the random distribution due to the development of a strong shear texture. Two disorientation angle ranges with high frequencies can be observed: below 15° and above 45° . The area fraction grain size distribution (Fig. 10c) indicates that the majority of grains are refined to sizes below $1 \text{ }\mu\text{m}$, as evidenced by several pronounced peaks within this range. Meanwhile, distinct peaks corresponding to larger grains are also present in the distribution. However, their area fractions are significantly lower than those associated with the fine-grain population. This confirms the non-uniform nature of the microstructure, in which a small number of larger grains coexist with a dominant fraction of ultrafine grains.

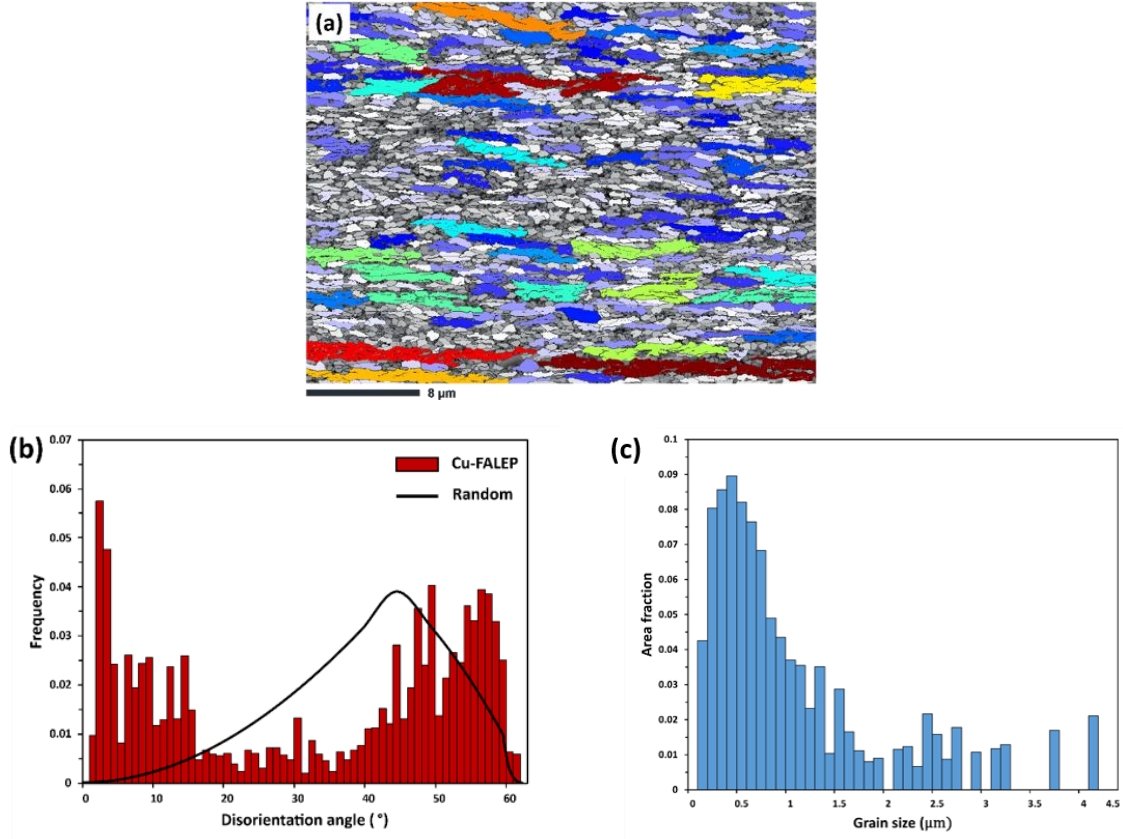


Fig. 10. (a) The microstructure of the Cu sample after the FALEP process with an extrusion ratio of 8.8 (The coloring is based on the grain sizes). **(b)** The corresponding next-neighbor disorientation distribution (bin size = 1°). The random Mackenzie distribution is shown by a solid black line. **(c)** The area fraction grain size distribution (bin size = $0.1 \mu\text{m}$).

To examine the relationship between grain size and crystallographic texture, the microstructure has been partitioned into two groups based on the grain size: larger grains and small grains. Grains above $2.15 \mu\text{m}$ are in the larger grains group (Fig. 11a), while grains below 620 nm are in the small grains group (Fig. 11b). The black regions in the partitioned microstructures are filtered. The larger grains exhibit an irregular morphology. It seems that they are formed by sticking some unpaired fragments. The small grains exhibit a nearly equiaxed, highly uniform morphology. The homogeneity and lack of elongated or irregular features suggest that these grains are already within, or very close to, the steady-state regime of grain size.

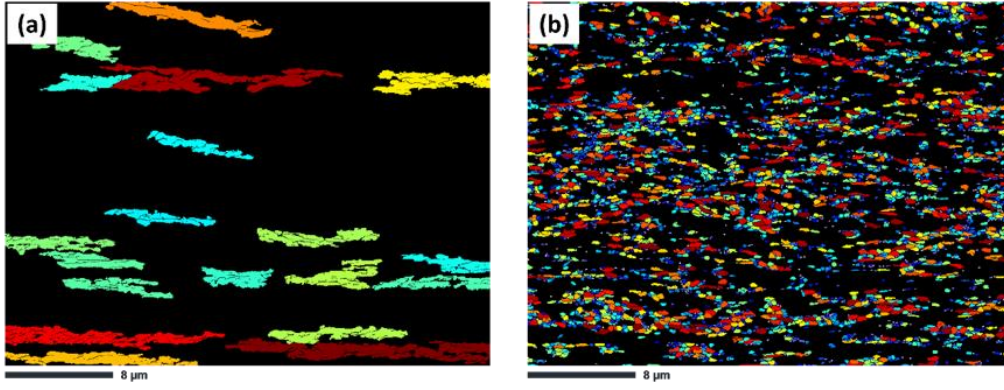


Fig. 11. The microstructure of the Cu-FALEP sample **(a)** larger grains, **(b)** small grains. The dark areas are filtered. The grains are colored according to the grain size scale.

Fig. 12a presents the orientation distribution function (ODF) sections of the measured texture for the Cu-FALEP sample in the $\varphi_2 = 0^\circ$ and 45° sections of Euler space. The locations of the ideal shear texture components are also indicated in these sections. These ideal orientations were calculated based on the simple shear model. However, in the FALEP experiment, the position of the shear plane was located 14° away from the x-axis, which was determined from the ideal shear fibers observed in the measured texture. Therefore, they are presented at their 14° rotated position in the experimental textures. This angle is much larger than the position of the assumed ideal shear plane, which was 6.48° . According to Fig. 12a, after the FALEP process, a typical shear texture is observed, with the C component showing the highest intensity, followed by the B and A1 components. Furthermore, some grains rotated along the rotated-cube fiber ($\phi = 0^\circ$ line), leading to the appearance of this non-ideal shear fiber. The ODF sections after microstructure partitioning for the larger and small grain groups are shown in Figs. 12b and c. By comparing the textures of larger and small grains, a clear and significant trend can be observed. Larger grains are almost always in the vicinity of the ideal shear positions, while small grains are spread out in a wider range of orientation space. Small grains do not always occupy near ideal positions. Moreover, the maximum texture intensity for larger grains is around 56, which is quite higher than that of small grains (10.8). A quantitative comparison of the two grain-size groups further highlights their distinct orientation characteristics. The volume fraction of the individual ideal shear components, as well as the combined volume fraction of all ideal components, was calculated using a 20° disorientation threshold around the ideal positions, and the results are presented in Fig. 12d. As can be seen, more than 90% of the large grains are in the vicinity of the ideal positions. For the small grains, the volume fraction of ideal shear components is about 76%, indicating that a larger portion of the refined grains occupies non-ideal positions in the orientation space.

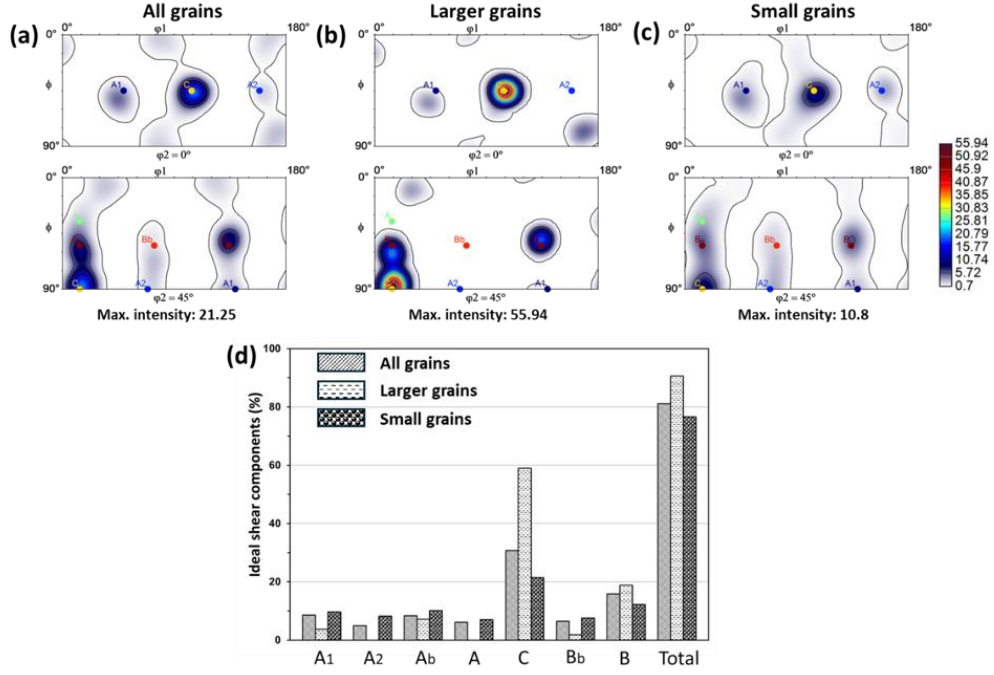


Fig. 12. ODF sections of the Cu-FALEP sample measured texture at $\varphi_2 = 0^\circ$ and 45° : (a) all grains, (b) larger grains, (c) small grains, and (d) the corresponding volume fractions of ideal shear components. The ideal positions are rotated by 14° around the TD axis to coincide with the experimental ideal positions.

2.4. Fractal Grain Refinement Model

The grain refinement model in Ref. [15] has been further developed and applied in this study to simulate the grain fragmentation and coalescence mechanisms. The original model used a 3-level fractal approach for grain fragmentation. At each level, a grain consists of two distinct zones: (i) the central zone, unaffected by the grain boundary, and (ii) the zone near the grain boundary. The lattice rotation rate in the grain boundary zone is assumed to be slower due to boundary pinning effects. Since the boundary and central zones are assumed equal in size, the grain resembles to a $3 \times 3 \times 3$ “Rubik cube”, if the initial grains are considered to have cuboidal shapes. In this model, except for the central sub-cube, all other sub-cubes have different numbers of external grain boundaries depending on their position; they are considered as subgrains. Each boundary is adding a contribution to the slow-down of the lattice rotation of the subgrain. The number of grain boundaries can be $k = 1, 2$, or 3 : 1 on the facet of the cube, 2 on an edge, and 3 at a corner position. The rotation distortion caused by these grain boundaries in a subgrain is represented by a rotation around the resultant grain boundary normal $\underline{n}_{GB}^{(res)}$. The latter is calculated as the vectoral sum of the grain boundary normal vectors $\underline{n}_{GB}^i$:

$$\underline{n}_{GB}^{(res)} = \sum_{i=1}^k \underline{n}_{GB}^i \quad (3)$$

Accordingly, the portion of the lattice rotation rate that arises from grain boundary effects is expressed as:

$$\dot{\underline{\Omega}}_{SG}^{GB} = -\text{sign}[\dot{\underline{\Omega}}_G \underline{n}_{GB}^{(res)}] |\sin \alpha| |\mu \dot{\underline{\Omega}}_G| \frac{\underline{n}_{GB}^{(res)}}{|\underline{n}_{GB}^{(res)}|} \quad (4)$$

Here, α is the angle between the resultant grain boundary normal of the subgrain $\underline{n}_{GB}^{(res)}$ and the lattice rotation rate vector of the parent grain $\dot{\underline{\Omega}}_G$. During plastic deformation, this angle evolves because the directions of both vectors change continuously. The grain boundary induced slow-down in the lattice rotation rate of the subgrain ($\dot{\underline{\Omega}}_{SG}^{GB}$) is then superimposed on the lattice rotation rate of the parent grain. The overall lattice rotation rate of the subgrain is thus:

$$\dot{\underline{\Omega}}_{SG} = \dot{\underline{\Omega}}_G + \dot{\underline{\Omega}}_{SG}^{GB} \quad (5)$$

2.5. Grain Refinement Simulation

The 4-level grain refinement model has been employed to simulate the evolution of the grain structure during simple shear deformation. Three different initial orientations were selected for analysis, and their corresponding Euler angles are listed in Table 2. Each orientation was assigned an identical initial volume fraction, meaning that the starting 2D and 3D grain sizes were the same for all cases. For polycrystal plasticity calculations, the Taylor model was used, with the only non-zero velocity gradient component of $L_{12} = -\dot{\gamma}$, corresponding to the negative simple shear in the shear reference system. For all simulations, the 12 $\{\bar{1}11\}\langle 110 \rangle$ slip systems were used with the slip-viscosity parameter of $l/m = 8$. The lattice curvature coefficient (μ) was set to 0.5 in all following simulations.

Table 2. The Euler angles and grain sizes of three initial grains used in the grain refinement simulation.

Grain ID	Euler angles (°)			Grain volume (μm^3)	Grain size 2D (μm)	Grain size 3D (μm)
	φ_1	Φ	φ_2			
Grain A	5	45	0	14420	27.46	30.19
Grain B	95	45	0			
Grain C	0	0	0			

Fig. 13 presents the 2D and 3D grain size evolution of Grain A and Grain B during the deformation up to an equivalent strain of 4.61 (shear strain of 8). The volume-weighted average

grain size of Grain A significantly decreased from 30.19 μm to 9.1 μm up to $\epsilon_{eq} = 3.6$ through successive grain fragmentation events. Interestingly, upon further deformation, the average 3D grain size remarkably increases to 21.14 μm at an equivalent strain of 4.61. This transition indicates that while fragmentation dominates at lower strains, grain coalescence becomes dominant beyond a strain of approximately 3.6, demonstrating that coalescence plays a significant role in the grain refinement behavior of Grain A at higher strains. A similar trend is apparent in the evolution of 2D grain size. The smallest area-weighted average grain size of 5.2 μm is achieved at $\epsilon_{eq} = 4$, after which the grain size increases to 9 μm at $\epsilon_{eq} = 4.61$. The 3D grain size evolution of Grain B (Fig. 13b) exhibits a sharp decrease at $\epsilon_{eq} = 0.8$, followed by a rapid increase in grain size at $\epsilon_{eq} = 0.9$. Similarly, the 2D grain size curve also shows a pronounced reduction in grain size at low strains. However, the extent of coalescence captured in the 2D analysis is less significant than in the 3D case, resulting in a sharp difference in grain size between the two representations near $\epsilon_{eq} = 1$. By further straining up to $\epsilon_{eq} = 4.61$, both the 2D and 3D analyses show a continuous decrease in grain size. At higher strain levels, limited grain coalescence occurs, which in turn acts as a compensation mechanism for grain fragmentation and locally reduces the rate of grain size decline. Unlike Grain A, however, no considerable grain size increase is observed for Grain B at high strains.

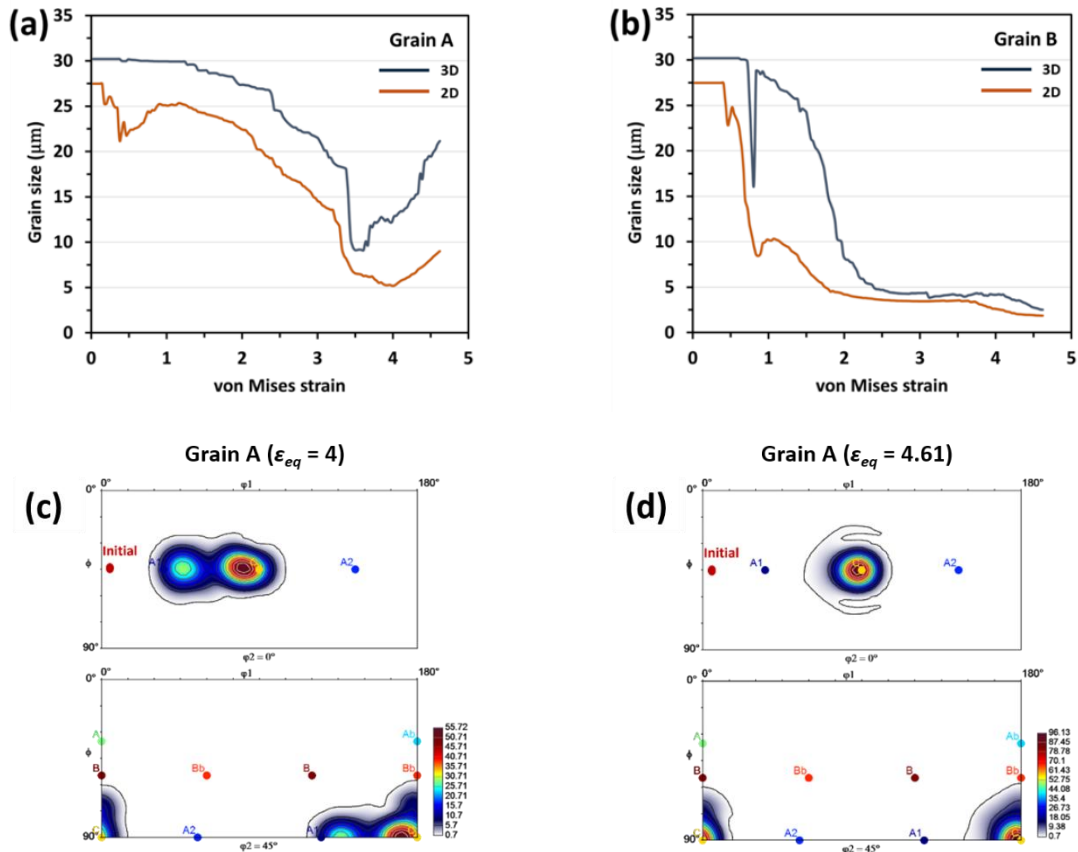


Fig. 13. The 2D and 3D grain size evolutions of (a) Grain A, and (b) Grain B simulations during simple shear deformation up to $\varepsilon_{eq} = 4.61$. $\varphi_2 = 0^\circ$ and 45° ODF sections of the simulated textures of (c) Grain A at $\varepsilon_{eq} = 4$, (d) Grain A at $\varepsilon_{eq} = 4.61$

Another output of the present model is the crystallographic texture. Figs. 13c and d show the simulated textures for Grain A at $\varphi_2 = 0^\circ$ and 45° sections of Euler space. To evaluate the influence of texture evolution on the fragmentation and coalescence behavior of Grain A, two deformation stages were examined: $\varepsilon_{eq} = 4$ (Fig. 13c), where the fragmentation rate has begun to decrease, and $\varepsilon_{eq} = 4.61$ (Fig. 13d), where significant grain coalescence has occurred. At $\varepsilon_{eq} = 4$, two distinct orientation clouds are observed: one located after the A1 component and another with a higher intensity before the C component. When the strain reaches 4.61, the two orientation clouds merge into a single cloud with a very high intensity at the ideal C orientation. This indicates that grain coalescence for Grain A predominantly occurred at the ideal C position.

Grain C was initially located on the rotated-cube fiber. Orientations on the rotated-cube fiber resist rotating toward ideal shear orientations and regions with high convergence/divergence fields. The 2D and 3D grain size evolutions of Grain C during deformation up to $\varepsilon_{eq} = 4.61$ are shown in Fig. 14. The 3D grain size evolution displays different stages, in which significant grain coalescence occurs. This trend can also be observed in 2D grain size analysis, but with lower intensity. At first glance, the occurrence of grain coalescence for an initial cube orientation may appear unexpected, since this orientation is known to resist rotation toward the ideal shear positions, where coalescence is typically activated. However, local convergence fields can play key roles in grain coalescence along the rotated-cube fiber. Figs. 14b and c present the simulated textures of Grain C at two different strains, $\varepsilon_{eq} = 3.8$ and $\varepsilon_{eq} = 4.61$, corresponding to states before and after the final coalescence stage, respectively. At $\varepsilon_{eq} = 3.8$, the initial cube orientation appears to have completed a full cycle of rotation along the rotated-cube fiber, returning to the cube position. During fragmentation, however, a fraction of grains deviates from the rotated-cube fiber due to the local divergence fields (intragranular misorientation) introduced by CDRX. This allows them to reach regions close to several ideal shear orientations, such as A1, B, and Bb. With further straining up to $\varepsilon_{eq} = 4.61$, some grains rotate toward the ideal C orientation. At the same time, the intensity of ideal A1, B, and Bb components decreases. Nevertheless, the rotated-cube texture remains the dominant component at both deformation stages. Moreover, the maximum texture intensity increases to 83 at the final strain level, and the orientation cloud near the rotated-cube fiber becomes more localized. These observations indicate that the increase in grain size of Grain C at $\varepsilon_{eq} = 4.61$ is

driven predominantly by grain coalescence around the rotated-cube fiber, rather than by coalescence occurring near the ideal shear orientations. This observation indicates that the rotated-cube texture represents a special case in simple shear deformation with respect to grain fragmentation and coalescence behavior, where grain coalescence is driven by local convergent fields far from ideal shear components.

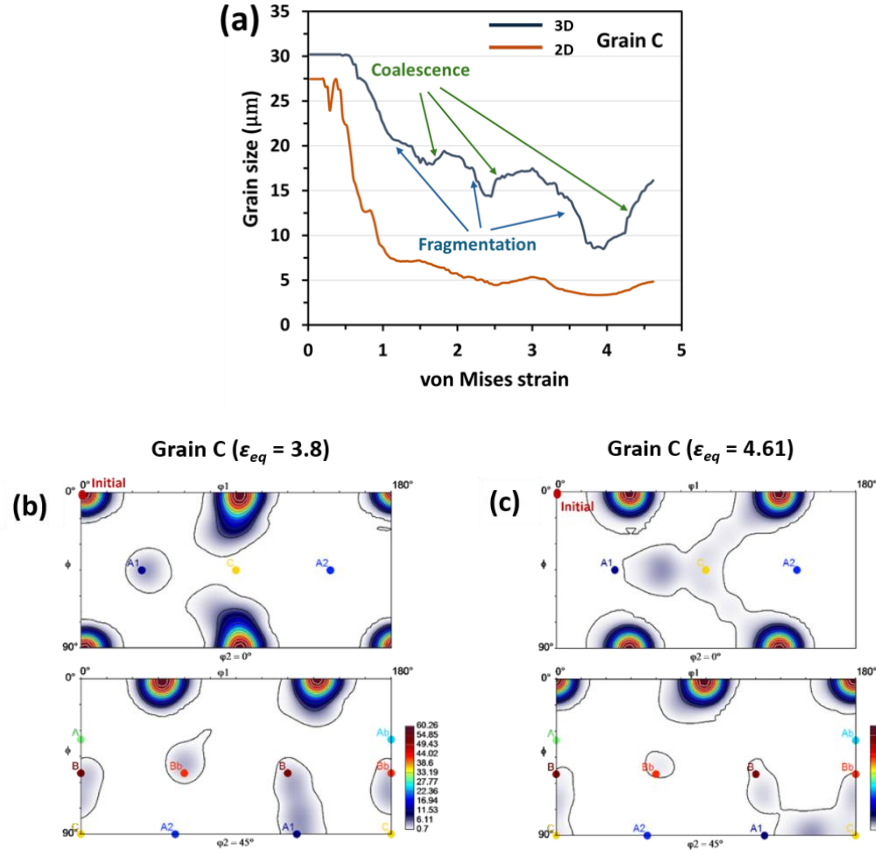


Fig. 14. (a) The 2D and 3D grain size evolutions of Grain C simulation during simple shear deformation up to $\varepsilon_{eq} = 4.61$. $\varphi_2 = 0^\circ$ and 45° ODF sections of the simulated textures of Grain C at (b) $\varepsilon_{eq} = 3.8$, and (c) $\varepsilon_{eq} = 4.61$.

Scientific Claims

1. Gradient microstructure formation in FALEP

It has been experimentally demonstrated that FALEP processing of Al-1050 alloy can produce a gradient microstructure across the sheet thickness at almost half (10.5) the previously published extrusion ratio (20). EBSD results show an average grain size of 720 nm near the top surface and 4.2 μm near the bottom surface, with distinct crystallographic textures in the two regions.

2. Deformation field and texture analysis in FALEP using a new three-stage flow line model

The deformation behaviour of the experimental flow lines after the FALEP process at an extrusion ratio of 10.5 exhibits some sharp variations. Three deformation stages can be identified, including two simple shears and a linear convergent extrusion stage in between. This complexity in flow line deformation was not observed in previous studies of other channel angular extrusion processes, such as ECAP and NECAP. The classic simple shear model of angular extrusion fails to predict the strain and deformation field

in the FALEP process at an extrusion ratio of 10.5. The simple shear model assumes uniform deformation across the sheet thickness, which makes it impractical for modeling gradient microstructures. While the simple shear model approaches reasonably well at higher extrusion ratios (20), it overestimates the strain at lower extrusion ratios (10.5). The simulated textures generated by the simple shear model are in poor agreement with the measured textures for both the top and bottom regions. Therefore, the simple shear approximation is only applicable at high extrusion ratios (≈ 20), but becomes invalid at lower ratios, where deformation heterogeneity and gradient microstructure develop. Using 2D fluid mechanics kinematics, a new three-stage flow line model has been developed to compute local velocity gradient tensors. When coupled with a polycrystal plasticity framework, the model successfully reproduces experimentally measured textures with accuracies of 86.3 % (upper region) and 77.3 % (bottom region). This confirms that the proposed model can accurately describe the deformation mode and predict the resulting texture evolution in FALEP.

3. The critical role of texture evolution in grain refinement: fragmentation vs coalescence

- 3.1.** Grain refinement during plastic deformation is not a one-way process. Indeed, the final grain size results from two competing mechanisms: grain fragmentation and grain coalescence; both are strongly dependent on texture evolution. A commercially pure copper sample after the FALEP process exhibited a microstructure consisting of many small grains together with some larger grains. Larger grains were formed through dynamic grain coalescence and showed ideal shear orientations. The driving force of grain coalescence is the convergence field of texture evolution in which the disorientation between neighboring grains gradually decreases. In the vicinity of ideal orientations, the orientation difference can be smaller than the grain boundary detection angle. Therefore, the grain boundary disappears, and the grains are merged. In contrast, the divergence field of texture evolution increases the misorientation between the adjacent subgrains, promoting their transformation into new high-angle boundaries and thus grain fragmentation.
- 3.2.** In the context of continuous dynamic recrystallization during severe plastic deformation, grain coalescence is expected to occur when the following conditions are satisfied:

- Neighboring in physical space
- Neighboring in orientation space
- Approaching the ideal positions in orientation space

Coalescence is possible for those grains that have common grain boundaries, meaning that they are neighbors. Moreover, the neighboring grains that have large orientation differences are not suitable candidates for grain coalescence. Therefore, the neighboring condition should also exist in the orientation space, meaning that the disorientation between the grains is not too sharp. Furthermore, coalescence is only permitted near the ideal orientations, where the rotation field is convergent, and the lattice rotation rate is low. Continuous dynamic recrystallization (CDRX) inherently satisfies the first two conditions as the fragmented grains are physically adjacent and their orientations are correlated with the original grain orientation, meaning they are also neighbors in the orientation space. Coalescence is therefore activated only when the third condition is reached, i.e., when the grains enter a convergent rotation field and reach near the ideal positions. This demonstrates that grain coalescence is an intrinsic stage of the CDRX mechanism driven by texture evolution.

3.3. The rotated-cube fiber is an exception in grain coalescence theory. Although no individual orientation along this fiber is stable, when the whole fiber is considered, it exhibits a form of relative stability during simple shear deformation. Despite being located far from the ideal shear positions in Euler space, grain coalescence can still occur along the rotated-cube fiber. The driving force for grain coalescence along the rotated-cube fiber is the local convergence fields generated by internal misorientation gradients. The weak external convergence/divergence fields along the rotated-cube fiber keep the orientation evolutions within a narrow Euler space zone. As a result, the role of local convergence/divergence fields in grain fragmentation and coalescence along the rotated-cube fiber becomes pronounced.

4. Fully quantitative 3D and 2D grain fragmentation and grain coalescence analyses by an optimized 4-level grain refinement model

An existing 4-level grain subdivision model was extended by implementing 3D and 2D grain detection algorithms. For the first time, the model enables the detection of grains and the determination of grain size in both 2D and 3D at each strain level by considering

the topological connections between grains in physical space. From the outputs of this model, the following analyses can be done:

- Number of grains in 3D
- Average grain size in 2D and 3D
- Grain size distribution
- Number of fragmented and coalesced boundaries
- Deformation texture
- Disorientation distribution
- Microstructure simulation

The simulation results reveal that the 3D grain size is systematically larger than its 2D projection because neighboring grains may remain connected in the third direction, a factor typically neglected in EBSD-based 2D characterizations. Using the new model, quantitative analysis of grain fragmentation and grain coalescence is possible. The simulation results show that grain coalescence occurs near the ideal orientations, where the rotation field is convergent, and the lattice rotation rate is minimal, with the exception of the rotated-cube fiber. Moreover, the initial orientation plays a critical role in the level of grain fragmentation and grain coalescence. Under the same deformation conditions, different initial orientations can result in significantly different final grain sizes, indicating that the nature of texture evolution is a crucial factor in grain refinement.

Publications and Presentations

1. **Amininejad, A.**, Toth, L. S., Sepsi, M., Szucs, M., Kumaran, S. N., and Mertinger, V. (2025). Deformation field and texture analysis in friction-assisted lateral extrusion of aluminum. *Materials Characterization*, 223, 114920.
2. **Amininejad, A.**, Toth, L., and Mertinger, V. (2025). Modeling of deformation mode in ECAP variant techniques. *Doktorandusz Almanach*, vol. 1.
3. **OATK 2023**, Modeling of deformation field in the friction-assisted lateral extrusion process. **Amininejad, A.**, Sepsi, M., Szucs, M., Toth, L. S., and Mertinger, V. Poster Presentation.

4. **ICOTOM 2024**, A new flow line approach for modeling the deformation field and texture in FALEP. **Amininejad, A.**, Toth, L. S., Mertinger, V., Szucs, M., and Sepsi, M. Oral Presentation.
5. **ISCAME 2024**, On the role of crystallographic texture in grain fragmentation during severe plastic deformation. **Amininejad, A.**, Szucs, M., Toth, L. S., and Mertinger, V. Oral Presentation.

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