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Microstructure prediction using finite element simulation and artificial neural network for extrusion of AA6XXX aluminum alloy

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Abstract. Grain size evolution in AA6XXX extruded profiles is a critical factor influencing their mechanical, thermal and surface properties. Traditional techniques for microstructure control are often resource-intensive and time-consuming. This study presents an innovative approach that combines Finite Element Method (FEM) simulation with experimental microstructure measurements to train an Artificial Neural Network (ANN) for grain size prediction. A hollow AA6060 profile was extruded and experimentally characterized to determine its grain size distribution. Experimental data were compared with the results of FEM simulations conducted using QForm Extrusion UK software. Based on this comparison, an ANN was trained using the FEM outputs as input data to predict the final microstructure of the extruded profile. The proposed methodology demonstrated good accuracy in predicting the microstructure through the use of FEM simulations and machine learning techniques. This approach provides a faster, more sustainable and more cost-effective alternative to conventional methods, representing a significant advancement in optimizing the extrusion process for AA6XXX alloys.

Introduction

The extrusion of AA6XXX series aluminum alloys is crucial for the automotive industry, where lightweight, high-performance materials are essential to meet strict standards for mechanical strength, formability and corrosion resistance [1]. Achieving optimal properties in extruded profiles requires precise control of the microstructure, which is influenced by factors such as alloy composition, extrusion parameters and heat treatments. One of the key challenges is controlling microstructural evolution, which directly impacts the mechanical and crashworthiness properties of the material, potentially compromising the suitability of profiles for automotive applications. [2–5].

The prediction of microstructural evolution in aluminum alloys during extrusion has seen significant progress through the integration of FEM simulations with analytical and empirical models. FEM-based approaches are particularly adept at capturing the spatial distribution of the temperature, strain and strain rate during extrusion [6]. Coupled with recrystallization models, they can predict grain refinement and Peripheral Coarse Grain (PCG) formation with moderate accuracy [7]. Analytical models, often based on classical theories of plastic deformation and heat transfer, complement FEM simulations by providing closed-form solutions for simpler geometries and process conditions [8]. Recent studies have highlighted the benefits of hybrid approaches, where FEM simulations provide high-fidelity process data, which is then utilized in analytical frameworks to enhance computational efficiency [9–11]. Despite these advances, challenges remain in scaling these models to complex industrial setups, especially for hollow profiles with intricate die geometries and multi-stage thermal cycles.

The complexity of the relationship between extrusion conditions, PCG formation and grain size distribution suggests the potential for data-driven modeling to improve predictions. Machine learning (ML) algorithms are particularly suitable for multidimensional problems with low transparency, making them an effective tool when combined with analytical and numerical models for predicting grain size during hot extrusion. ML has been widely applied in manufacturing, showing significant improvements over traditional models. For example, Cui et al. [12] used a backpropagation neural network (BPNN) combined with a genetic algorithm to predict softening kinetics and rolling forces in steel rolling processes. In extrusion, early works like those by Hsiang et al. [13] and Zhou et al. [14] demonstrated the potential of artificial neural networks (ANN) for predicting extrusion load, exit temperature and material behavior, with results in alignment with FEM simulations. More recent applications, such as the combined FEM/ANN approach, have shown promising results for predicting the grain size distribution in extruded profiles, achieving reasonable accuracy with limited datasets [15]. While these data-driven approaches show great promise, challenges remain. The available datasets are often limited and the generalization of models across different materials and extrusion conditions is still a work in progress. Furthermore, combining ML models with FEM simulations requires substantial computational resources, while the robustness of models needs further validation through more extensive experimental data.

This study combines Finite Element Method simulations with an ANN to predict microstructural outcomes during extrusion. FEM simulations provide detailed insights into strain, strain rate, temperature and recrystallization kinetics, while the ANN recognizes patterns and correlations within multidimensional datasets. By combining these approaches, the present work aims to develop a robust methodology for predicting grain size evolution in AA6060 extruded profiles. A hollow AA6060 profile was selected as the case study, with experimental characterization performed to determine the grain size distribution. FEM simulations conducted using QForm Extrusion® software provided a comprehensive dataset of process variables, serving as inputs for training the ANN. The results demonstrate that the proposed FEM-ANN framework can accurately predict the final microstructure, offering a potentially faster and more cost-effective alternative to traditional experimental methods. This approach not only enhances the understanding of grain size evolution but also provides a practical tool for optimizing extrusion processes, contributing to the development of advanced aluminum alloy profiles tailored to automotive applications.

Experimental Procedure

The experimental campaign was based on a previous work analyzing a hollow profile in AA6060 alloy [8], extruded by Profilati SpA in Medicina, Italy. During the production batch, 17 billets were extruded, with data regarding the profile exit temperature and extrusion load collected throughout the process. These measurements were utilized to validate numerical simulation results. The extrusion process was conducted with a ram speed of 8 mm/s and an extrusion ratio of 27. The container, billet and die temperatures were set to 430°C, 480°C and 510°C, respectively. The ram acceleration phase lasted 5 seconds. Each billet measured 950 mm in length and 203 mm in diameter, while the container had a diameter of 211 mm. After extrusion, a rest length of 44 mm was left for each billet.

Detailed analysis of the extruded profile obtained with the seventh billet was performed to ensure that steady-state conditions were achieved within the tool-die system. Specimens were

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extracted from the central section of the extruded profile, corresponding to a ram stroke of 475 mm, to ensure representative measurements. In order to investigate the microstructure of the profile, samples underwent grinding, polishing and electrolytic etching. Polarized light microscopy (Zeiss AXIO) was used to capture images of the etched surfaces, with the average grain size determined in line with ASTM-E112. The sample under investigation was extracted from the central section of the extrusion profile, corresponding to a ram stroke of 475 mm. Data obtained from measurements performed on the extracted profile were used to construct a dataset consisting of approximately 500 entries, which served as the training set for the ANN. These data represent the output values of the ANN during the training phase, corresponding to the grain size to be predicted based on specific input parameter combinations. Details regarding the input parameters are discussed in the following section.

FEM Simulation

Simulation of the extrusion process was performed in Qform Extrusion UK, a commercial finite element (FE) software based on the Arbitrary Lagrangian-Eulerian (ALE) approach. The thermal and mechanical properties of the employed AA6060 aluminum alloy were defined to accurately replicate the behavior of the material during the extrusion process. These properties, listed in Table 1, included density, specific heat, thermal conductivity, thermal expansion, Young's modulus and Poisson's ratio. The flow stress of the AA6060 alloy was modeled using the Hensel-Spittel constitutive equation (Eq. 1), which is widely used for representing the thermo-mechanical behavior of materials under extrusion conditions. This model describes the material flow stress as a function of strain, $\bar{\varepsilon}$, strain rate, $\dot{\boldsymbol{\varepsilon}}$, and temperature, T, based on the nine material constants reported in Table 1. These constants (A, m_1 to m_9) were sourced from the Qform database for AA6060 alloy.

$$\bar{\sigma} = A \cdot e^{m_1 T} \cdot \bar{\varepsilon}^{-m_2} \cdot \dot{\varepsilon}^{-m_3} \cdot e^{\frac{m_4}{\bar{\varepsilon}}} \cdot (1+\bar{\varepsilon})^{m_5 T} \cdot e^{m_7 \bar{\varepsilon}} \cdot \dot{\varepsilon}^{m_8 T} \cdot T^{m_9}, \quad (1)$$

AA6060	Parameters	Values
Thermal and mechanical properties	Density [kg/m^3]	2690
	Specific heat [J/kg K]	900
	Thermal conductivity [W/m K]	200
	Thermal expansivity [m/K]	2.34×10^{-5}
	Young's modulus [GPa]	68.9
	Poisson's ratio	0.33
Flow stress Hensel-Spittel material constants	A [MPa]	280
	m1 [K^{-1}]	-0.00461
	m2	-0.16636
	m3	0.12
	m4	-0.02056
	m5 [K^{-1}]	0.00036
	m7	0
	m8 [K^{-1}]	0
	m9	0

Friction conditions between the billet and tool were modeled based on the optimized default settings provided within Qform. Sticking conditions were assumed for most interfaces (billet-container, billet-ram and billet-die), while the Levanov friction model was applied to the bearings, with parameters m = 0.3 and n = 1.25 [1].

In order to validate simulation outputs, the predicted extrusion load and profile exit temperature were compared to experimental values. The experimental peak extrusion load was recorded as 23.4 MN, while the simulated value was 23.3 MN, resulting in an error of less than 1%. Similarly, the experimental exit temperature, measured with a pyrometer at the die exit, was 557°C, compared to the predicted temperature of 562°C, yielding a prediction error close to 1%. Overall, the simulation demonstrated excellent agreement with experimental results, with an average error below 1% for both extrusion load and exit temperature, confirming the reliability of the numerical model.

Output parameters directly calculated or derived from the FEM simulation were strain, temperature, maximum strain rate, the Zener-Hollomon parameter, subgrain size and stored energy. Strain and temperature are standard parameters automatically computed by Qform Extrusion UK. The maximum strain rate was determined following the methodology outlined in [16] by analyzing strain rate values calculated at each time step along the deformation path from the billet to the profile and selecting the maximum value. The Zener-Hollomon parameter and stored energy were computed as described in the Negozio-Donati model [1], as detailed below (Eqs. 2 to 4):

$$\frac{1}{\delta} = C\,(lnZ)^n \tag{2}$$

$$Z = \dot{\varepsilon}_{max}\, exp\left(\frac{Q}{RT}\right) \tag{3}$$

$$\mathrm{Pd} = \frac{Gb^2}{10}\left[\rho_i(1\text{-}\ln(10b\rho_i^{0,5}))+\frac{2\theta}{b\delta} * \left(1+\ln\left(\frac{\theta c}{\theta}\right)\right)\right] \tag{4}$$

where Z is the Zener-Hollomon parameter, T is exit temperature, Pd is the stored energy, $C = 3.36\times10^{-9}$ m^{-1} and $n = 5.577$ are constants, Q is the activation energy of AA6060 (161000 J/mol·K [8]), R is the universal gas constant (8.341 J/mol), G is the material shear modulus (2.05×10^{10} Pa [8]) and b is the Burgers vector (2.86×10^{-10} m [8]). Moreover, $\dot{\varepsilon}_{max}$ represents the maximum strain rate, ρ_i the dislocation density, δ the subgrain size, Θ the misorientation angle and Θc the misorientation angle limit (15°).

Artificial Neural Network

The final dataset employed for training ANN models for predicting the grain size distribution within extruded profiles comprised the parameters described in the previous section as potential inputs and the experimental grain size as the output. Based on preliminary tests, final input parameters were selected as the strain, temperature, maximum strain rate, Zener-Hollomon parameter and stored energy, with correlated variables limited to those with complex non-linear functions. The entire dataset was partitioned into 80% training and 20% testing to allow the accuracy of the trained ANN to be assessed based on unseen data.

Training of ANNs for regression was performed with the *fitrnet* function in MATLAB. Grid hyperparameter optimization was carried out with Sigmoid, Hyperbolic tangent (tanh) and Rectified linear unit (ReLU) activation functions, 1-25 neurons per fully connected layer and 1-2 fully connected layers. The best combination of accuracy and generalization to unseen datasets was obtained with a Sigmoid activation function and two hidden layers, each with 20 neurons (Fig. 1). More complex ANNs were found to yield similar accuracy on average but with a greater tendency to contain outliers with no physical explanation. To assess the impact of each input variable on the calculated grain size, explainable machine learning was implemented by determining the permutation importance of each variable. Calculation of this parameter involved randomly shuffling one variable at a time and assessing the resulting reduction in model accuracy, with a greater reduction in accuracy indicating a greater importance of the input variable. The trained ANN was then employed to produce a predicted grain size map over the entire extrude profile based on FEM simulation outputs and the same derived microstructure-specific parameters to demonstrate visual outputs that could potentially be generated with automated ANN tools for microstructure prediction during extrusion.

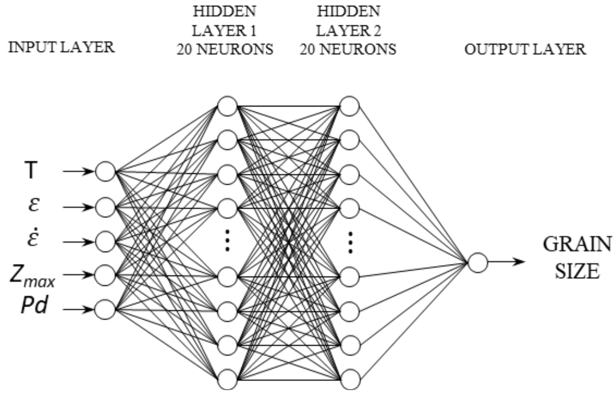

Figure 1 – Schematic of the ANN.

Results and Discussion

Unlike other 6XXX series alloys such as AA6082 or AA6061, AA6060 aluminum alloy undergoes rapid static recrystallization immediately after extrusion [2], which can be clearly seen in the fully recrystallized microstructure observed in the micrographs shown in Fig. 2, where the average grain size ranges from around 55 µm and to 125 µm.

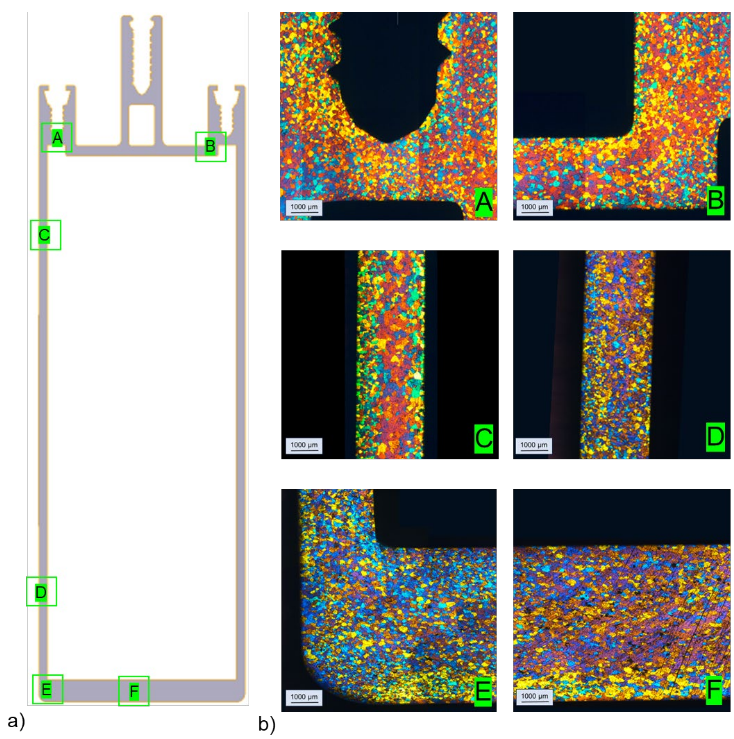

Figure 2 – a) Geometry of the extruded AA6060 profile, b) grain size analysis.

The results of the FEM simulation (Fig. 3) revealed that strain values and maximum strain rates were primarily within the ranges 0–50 and 20–1500 s^{-1}, respectively, with only a few instances exceeding these limits. The temperature was calculated to be approximately 560 °C across virtually the entire profile section. The Zener-Hollomon parameter ranged from 3.5×10^{16} to 1×10^{18}, while the Stored Energy ranged from 250 to 750 kJ/mol·K.

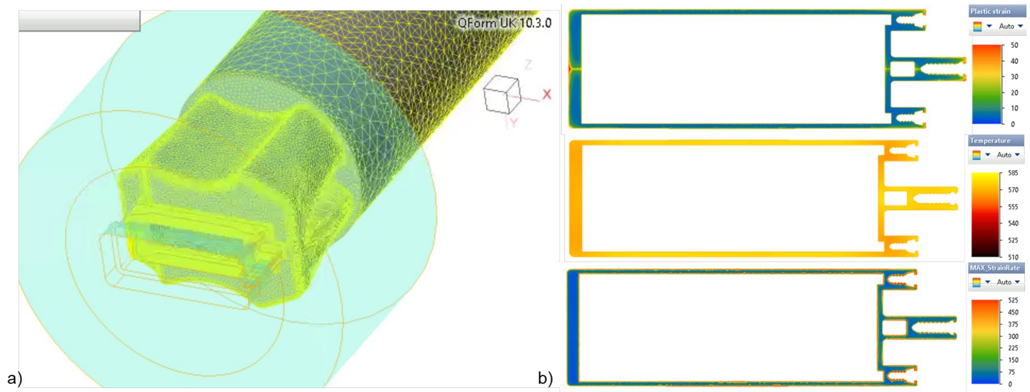

Figure 3 – a) Simulation of the extrusion process in Qform Extrusion UK, b) FEM outcomes in terms of strain, temperature and maximum strain rate.

After collecting data from the FEM simulation and cross-referencing them with experimental measurements of grain size, the training phase of the neural network was performed. The results of grain size prediction in the test dataset with the trained ANN are presented in Fig. 4, together with the mean importance of input parameters employed as predictors. The predicted grain size was close the true grain size (red line) in most cases, while the maximum variation generally remained within ±25% (blue dashed lines). The MSE was 75 μm^2, while the Mean Absolute Percentage Error (MAPE) was just 7.4%. These outcomes represent an improvement over existing analytical models for predicting the grain size of extruded profiles.

The mean importance of input parameters highlighted the significance of combining FEM simulations generating standard outputs with an analytical framework for calculating microstructure-specific parameters. The stored energy, Pd, was by far the most important parameter influencing model accuracy, followed by the temperature, T, strain, ε, maximum strain rate, $\dot{\varepsilon}_{max}$, and finally Zener-Hollomon parameter, Z. Lowest importance of the latter was likely due, in part, to its influence on the stored energy via the subgrain size, δ; however, it must be noted that the mean importance of Z was nonetheless significant, justifying its inclusion amongst the input parameters employed for training the ANN.

Fig. 5 presents a grain size map of the extruded profile generated with values obtained from the trained ANN model based on the aforementioned input parameters obtained with FEM simulations and analytical calculations. It can be observed that a larger grain size is predicted within internal regions of the profile, while grains tend to be smaller on average at the surface. The predicted range is from 60 to 115 μm. These outcomes are in general agreement with the experimental profile. It should be noted that additional experiments are required to validate this approach, which should include the extrusion of different profiles with various geometric characteristics and process parameters. However, the outcomes achieved in this study demonstrate how the employed approach represents a robust and practical framework for predicting grain size in extruded profiles.

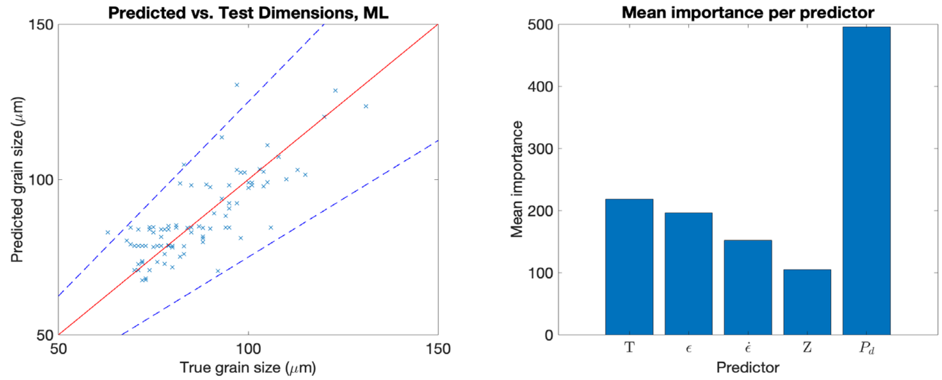

Figure 4 – Predicted grains size vs. true grain size in test set with trained ANN. Mean permutation importance of each input variable within the same model and dataset.

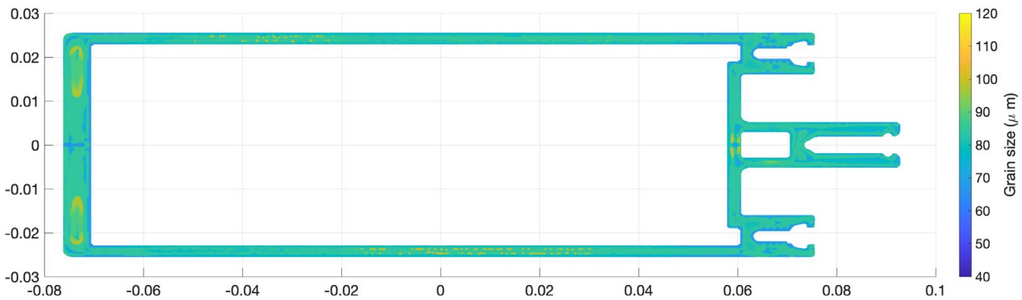

Figure 5 – Map of predicted grain size obtained with trained ANN model based on FEM simulation outputs and calculated microstructure-specific parameters.

Conclusion

While it is clear that more diverse datasets must now be employed for training ANNs capable of predicting various aspects relating to the microstructure of extruded profiles over a wider range of parameters, geometries and materials, machine learning within this field shows much promise in improving the capability and accuracy of predictive tools for forming processes. This, in turn, is likely to reduce resource requirements and cost associated with new configurations and products, as well as lead to higher quality products that can be more effectively optimized based on simulation and experimental data.

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