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Prediction of the Average Grain Size for AA5754 Plates and Sheets by Using Supervised Machine Learning

Maria STOICANESCU
Transilvania University of Brasov, Romania, stoican.m@unitbv.ro
Marin PETRE
ALRO SA, Romania, mapetre@alro.ro

Abstract
The enhancement of aluminium alloys mechanical properties can be achieved through the process of grain refinement. Grain size stands out as the primary indicative factor employed in industry to define grain refinement. This has led to a growing interest in the creation of precise models for predicting grain size. Methods rooted in data-focused informatics are gaining significance in assessing material properties that prove challenging to gauge or calculate through conventional means—often due to constraints related to cost, time, or labour. These methods leverage existing dependable data or have the potential to generate such data, particularly for essential scenarios. In this paper, several models are presented for predicting the average grain size of plate or sheet products made from AA5754, specifically in H111 or H22 tempers and with thicknesses ranging from 1 mm to 100 mm. These models are developed through regression analysis of empirical data, emphasizing the influence of factors like alloy composition, mechanical characteristics, and final product thickness. The findings underscore the efficacy of machine learning in constructing a data-oriented predictive model for grain size in AA5754.

Keywords
AA5754, average grain size, regression

1. Introduction

AA5754 is primarily composed of aluminum, with additional elements added to provide specific properties and characteristics. Its primary alloying element is magnesium (Mg), which contributes to its moderate strength, corrosion resistance, and weldability. It is often used in various applications where a combination of these properties is required.

Considerable attention is directed towards accurately forecasting solidification microstructure, with a specific emphasis on average grain size of aluminium alloys [1]. This focus has led to the creation of a multitude of predictive models.

In the last decade, the field of materials science has witnessed a substantial increase of interest and progress in the domain of machine learning (ML). Operating on a data-centric basis, ML has the capacity to assist individuals in extracting insights from data, forming connections, and rendering informed decisions. Furthermore, ML has found utility in tasks such as microstructure analysis, characterization, and design within the materials science domain [2 - 6].

Several distinct models for predicting grain size have been formulated over time, each customized to specific adaptation conditions. These models predominantly fall into three categories: (i) theoretical models constructed through physical or mathematical deduction under specific conditions and assumptions, (ii) empirical models derived from regression analysis of experimental data, and (iii) Deep Learning (DL) models which learn these relationships in a more flexible by processing vast amounts of data through layers of interconnected nodes in a neural network [7].

Lately, DL approaches have demonstrated superior performance compared to other ML methods in the field of materials science [8]. Despite their numerous merits, DL methods also come with inconvenience, the most notable being their opaque nature – like a black box, which could restrict a comprehensive understanding of the phenomena being studied [9]. Typically, a DL model involves thousands to millions of parameters, rendering the interpretation of the model and the direct extraction of scientific insights challenging. While a minimum sample size of around 100 is usually required for machine learning, DL demands a substantially larger dataset, at least 500 samples [10]. In our specific scenario for AA5754, the empirical model was developed using an approximate set of 150 samples.

This paper presents multiple predictive models aimed at estimating the average grain size of AA5754 plates and sheets, in H111 or H22 temper. These models are constructed using regression analysis applied to empirical data, placing emphasis on the impact of variables like alloy composition, mechanical properties, and the thickness of the final product. The results highlight the effectiveness of machine learning in constructing a predictive model grounded in data for estimating average grain size in the context of AA5754.

2. Dataset and features

2.1. Dataset

There were 153 sets collected from industrial experiments and organized into a dataset for the products of AA5754, where each set represents a finished product of plate or sheet type, H111 or H22 temper, with a thickness between 1 mm and 100 mm.

Each set of products was obtained following an industrial flow process, starting with the casting of slabs by the Direct-Chill process and continuing with the scalping of the slabs. Then, after the preheating treatment, each slab was subjected to the hot rolling, reducing its initial thickness of around 500 mm to a range between 7 mm or 8 mm, and 100 mm. A part of these product sets was subjected an annealing treatment to achieve the H111 temper. Instead, the remaining part of the products was subjected of cold rolling to achieve a thickness ranging from 1 mm to 5 mm, followed by a partial annealing treatment to attain the H22 temper. Alternatively, some products were subjected an annealing treatment with a slightly strain-hardened (less than H11) to achieve the H111 temper.

The alloying composition features were represented by five elements: Aluminum (Al), Magnesium (Mg), Manganese (Mn) and Silicon (Si). Thickness of the final product was chosen as parameter of process. Tensile yield strength (TYS), ultimate tensile strength (UTS), and fracture elongation (FE) were considered as pivotal features of the mechanical characteristics.

From a theoretical standpoint, the microstructure of an alloy encompasses a range of elements, including the uniformity of grain distribution, grain size, intensity of texture, degree of recrystallization, as well as the arrangement, dimensions, and volume of secondary phases. These attributes of microstructure ultimately govern the properties of the alloys. To summarize, the average grain size resulting from recrystallization plays a crucial role in defining the overall microstructure within the aluminium alloys. It arises as an outcome of the interplay among various factors and offers a comprehensive depiction of the microstructural attributes. Therefore, this study places its emphasis exclusively on the average grain size (AGS) as the central microstructural feature.

Table 1 presents definitions and the corresponding ranges for each of these features.

Table 1. Definitions and ranges of features

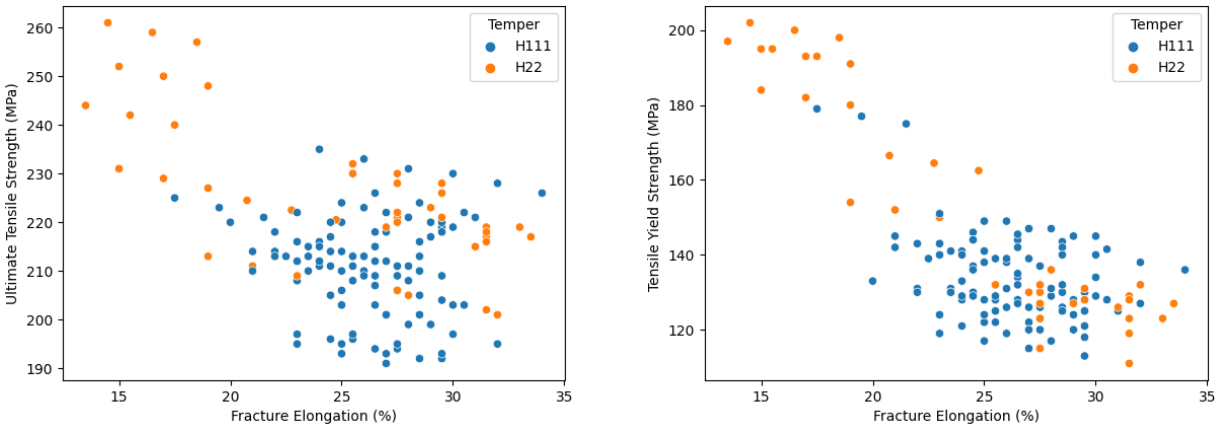
The feature group	Features	Range
Chemical composition	Al (wt. %)	95.3 – 96.5
	Mg (wt. %)	2.7 – 3.3
	Mn (wt. %)	0.1 – 0.5
	Si (wt. %)	0.2 – 0.40
Process parameter	Final thickness (mm)	1.0 – 100.0
Microstructure	Average grain size (μm)	12.9 – 205.9
Mechanical property	Ultimate tensile strength (MPa)	191 – 261
	Tensile yield strength (MPa)	111 – 202
	Fracture elongation (%)	13.5 – 34

Moreover, all these considered features can be found on any quality certificate that accompanies the products delivered to a customer, with the exception of the AGS, which is determined only for special applications or as a result of a specific customer's request.

Consequently, by developing the model presented here to estimate the average grain size, only the data from the quality certificates that accompany the products of the AA5754 type plates or sheets will be needed.

2.2. Relationships between features

A part of dataset was utilized to create Figure 1, where the vertical axis represents ultimate tensile strength (in MPa) or tension yield strength (in MPa), and the horizontal axis represents fracture elongation (in %). Figure 1 illustrates the correlation between the tempers (H22 vs H111) of the AA5754 and their corresponding mechanical properties. As anticipated, an enhancement in mechanical properties is noticeable for products in the H22 temper compared to those in the H111 temper. Additionally, mechanical property values for products in the H22 temper are dispersed along a diagonal line from the upper left to the lower right, whereas for products in the H111 temper, these values are predominantly clustered at the lower end of this line. This clustering suggests a trend of group.



a. The relationship between FE and UTS b. The relationship between FE and TYS

Fig. 1. Relationships between mechanical properties and tempers of AA5754

Much more eloquent is the representation of the data in the Figures 3 and 4 in the form of pair plots between the main elements of the chemical composition, final thickness, mechanical properties and average grain size for all data. Each individual subplot describes the relationship between two specific features.

We found that a strong correlation can be established between the final thickness and the average grain size of AA5754 products, H111 and H22 temper. For the other features, the data are much more dispersed and machine learning algorithms are needed that can handle dimensional and non-linear problems to find relationships between these features and to estimate the average grain size.

3. Modeling and results

All the figures and machine learning algorithms used in this study come from the scikit-learn library based on Python language [11].

The Pearson correlation coefficient was used to evaluate the importance of features influencing the average grain size. The results are shown in Figure 5.

A good correlation depends on the use, but it is safe to say you have at least 0.6 (or –0.6) to call it a good correlation. As can be seen from the coefficient's values for each feature, the most significant factor affecting the average grain size is the final thickness of the product, followed by content of silicon and fracture elongation. In contrast, the effects of Mn, Mg, Al, UTS and TYS on the average grain size are negligible.

The Pearson coefficient values can be explained by the fact that the most scattered data are the final thickness, and the least scattered are the mechanical properties and chemical composition, and in addition there are cases of products with different thicknesses but with the same chemical composition.

The following figures, Figures 6 – 9, show several models for predicting the average grain size of plate or sheet products made from AA5754, in H111 or H22 tempers and with thicknesses ranging from 1 mm to 100 mm.

Considering that in all four presented models the value of the Pearson coefficient is greater than or equal to 0.90, any of the models could be used to predict the average grain size of AA5754 products,

H111 or H22 temper. In addition, there is no point in including other features like chemical composition or mechanical properties in the prediction of the average grain size.

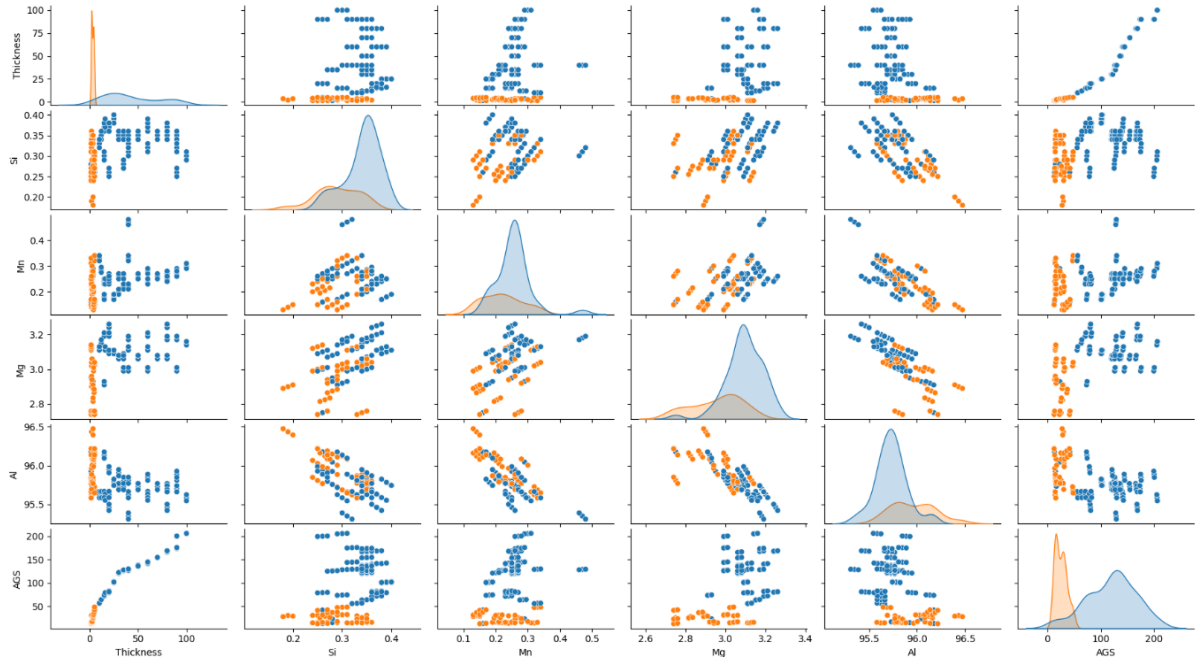


Fig. 3. Pair plots between the main elements of the chemical composition, final thickness, the average grain size and temper of AA5754

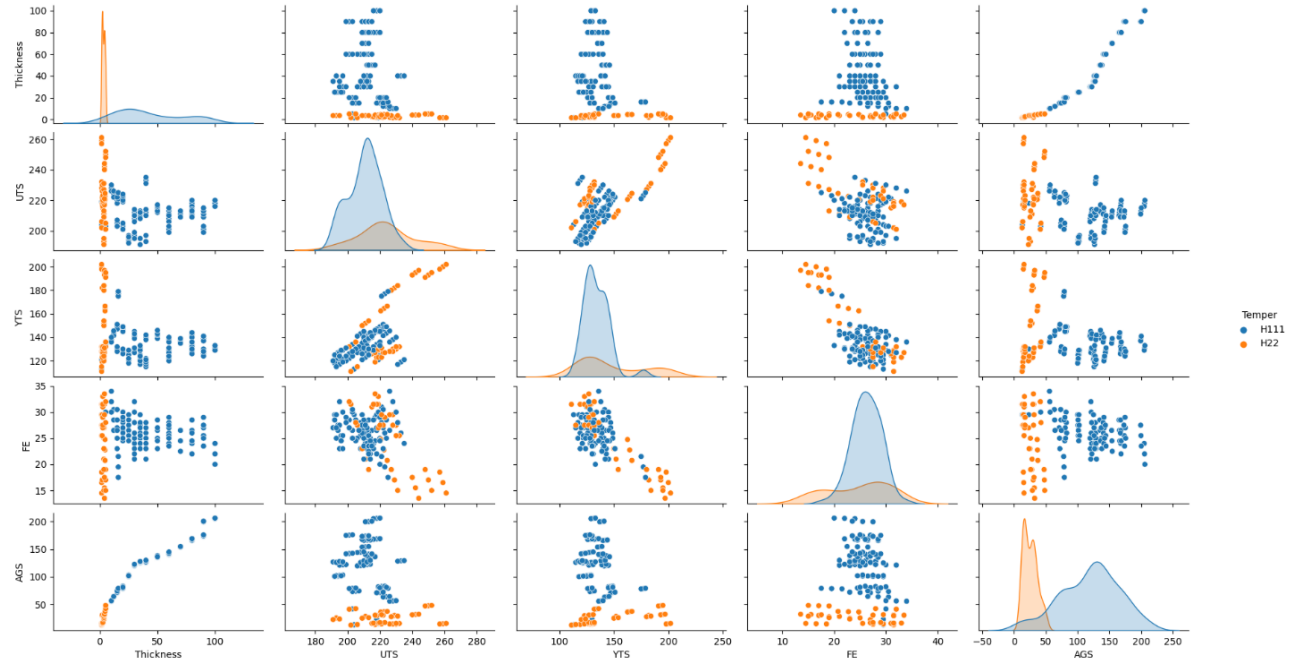


Fig. 4. Pair plots between final thickness, mechanical properties, average grain size and temper of AA5754 products

If a quick calculation of the average grain size is desired, then it is recommended to use the linear regression (Fig. 6). On the other hand, if the thickness of the AA5754 plate or sheet is greater than 1 mm and less than 80 mm, and a higher precision is desired, then it is preferable to use the logarithmic regression (Fig. 8). Finally, if the thickness is greater than 80 mm, then it is recommended to use the power or the exponential regression (Fig. 9).

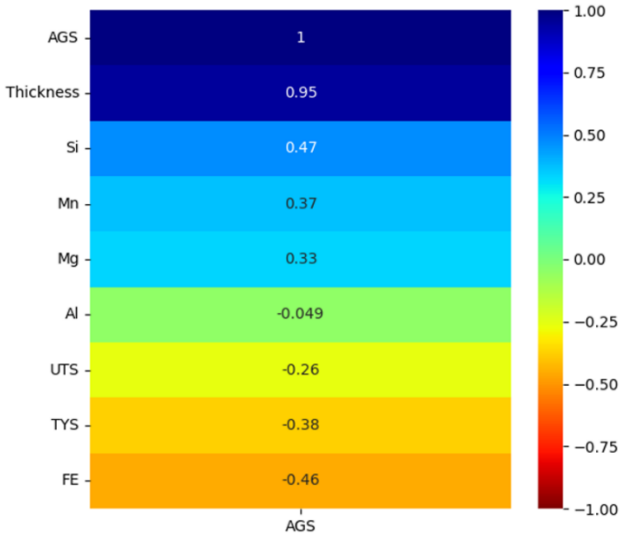


Fig. 5. The features correlating with average grain size of AA5754 products

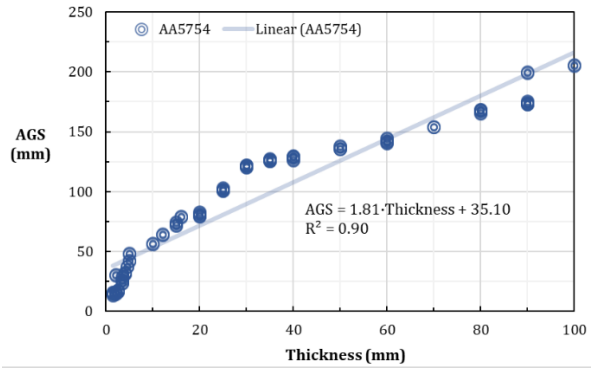


Fig. 6. Relationship between AGS and thickness of AA5754 by using linear regression

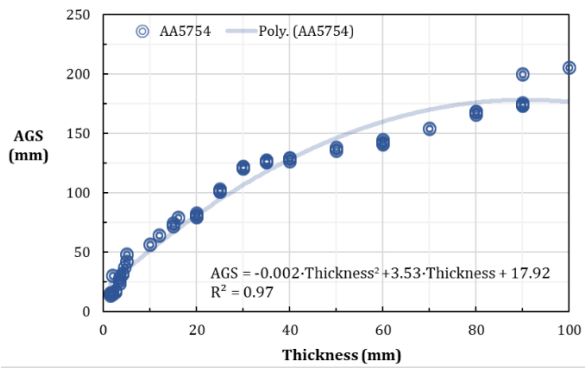


Fig. 7. Relationship between AGS and thickness of AA5754 by using 2nd polynomial regression

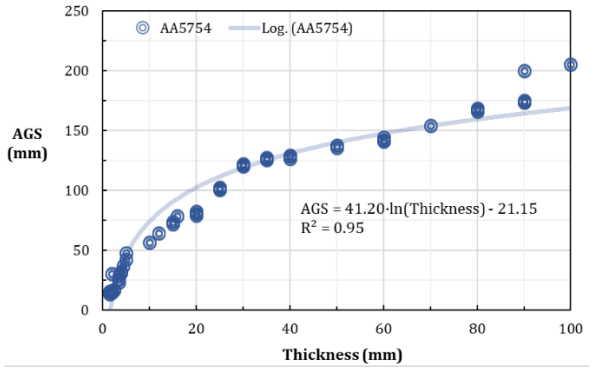


Fig. 8. Relationship between AGS and thickness of AA5754 by using logarithmic regression

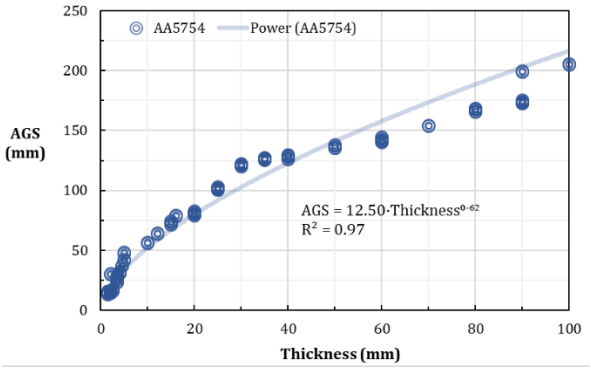


Fig. 9. Relationship between AGS and thickness of AA5754 by using power regression

Typically, exponential regression is used to model processes that grow slowly, then quickly, while logarithmic regression is used to model processes that grow quickly, then slowly.

Avoiding the utilization of polynomial regression (Fig. 7) is advisable, as second-order polynomial regression models tend to pose challenges in human interpretation. The increased complexity of these models diminishes the clarity around the factors that contribute to the predictions, ultimately influencing the accuracy of forecasts derived from such intricate models.

4. Conclusions

The improvement of mechanical properties in aluminium alloys can be accomplished by employing the technique of grain refinement. Within the aluminium industry, grain size is used as the principal parameter to define grain refinement. As a result, there has been an increasing focus on developing accurate models to predict grain size.

This study presents predictive models for estimating average grain size in AA5754 plates and sheets, H111 or H22 temper. Models are constructed via regression analysis using 153 sets of industrial data, considering alloy composition, mechanical properties, and product thickness (1 mm to 100 mm).

Final product thickness, Si content, and FE are the most influential factors for average grain size, while effects of Mn, Mg, Al, UTS, and TYS are minor.

All presented models with the input data of the final thickness and for which the Pearson coefficient is greater than or equal to 0.90 can be used to predict the average grain size of AA5754, H111 or H22 temper.

For quick calculations, it is recommended to use linear regression; and for more precise calculations, for thickness 1-80 mm, logarithmic regression, and for thicknesses greater than 80 mm, exponential regression. Finally, avoid polynomial regression because of the complexity and interpretation challenges that can affect forecast accuracy.

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