Supplementary information for

Interpretable machine learning analysis of stress concentration in magnesium: an insight beyond the black box of predictive modeling

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1. Elemental Features:

The features that have been are experimental data that have been obtained from the electron backscatter diffraction analysis (EBSD) of a Mg and AZ31 samples. Those features include the microstructural parameters, composition, strain, as well as geometric information about the grains (Table. S1)

Table S1. The elemental features that have been used in this work.

Feature category	**Feature**		
Geometric Features	X-axis		Y-axis
Microstructure parameters	Grain size (GS)	SF (Basal)	SF (1^{st} order <a> Pyr)
	Grain aspect ratio (GAR)	SF (<a> Prism)	SF (1^{st} order <c> Pyr)
	Misorientation (MO)	SF (<c> Prism)	SF (2^{nd} order <a+c> Pyr)
Stress/Strain parameters	Strain (%)		
Composition (at. %)	Mg	Al	Zr

2. Feature Transformations:

To enlarge the feature pool that is being used in this work, we have opted to use several mathematic transformations for the 16 elemental features mentioned above. Those transformations are; logarithmic transformation, squaring, cubing, cosine, sine, square root, exponential of the harmonic mean, and others. The following Table S2 shows the full feature list that have been used in this work:

Table S2. The full feature list (after the transformation process) that has been used in this work.

X-axis	GS	SF (1^{st} order <a> Pyr)	AR^3	$log\ AR$	$sin\ MO$	$\sqrt{MO}$	Total SF (TSF)	TSF^3
Y-axis	AR	SF (1^{st} order <c> Pyr)	GS^3	$exp(AR)$	$cos\ GS$	$asin(SF < Basal >)$	Average (SF)	$cos\ TSF$
Strain	MO	SF (2^{nd} order <a+c> Pyr)	MO^3	$exp[H(GS \times AR)]$	$cos\ AR$	$acos(SF\ (Basal))$	Median (SF)	$sin\ TSF$

Mg (at%)	AR^2	SF (Basal)	$log\ AR$	$exp[H(GS \times AR \times MO)]$	$cos\ MO$	$acos(SF(Basal))$	Range (SF)	$log\ TSF$
Al (at%)	GS^2	SF (<a> Prism)	$log\ GS$	$sin\ GS$	$\sqrt{AR}$	$acos^2(SF(Basal))$	Standard deviation (SF)	$exp(TSF)$
Zr (at%)	MO^2	SF (<c> Prism)	$log\ MO$	$sin\ AR$	$\sqrt{GS}$	$\sqrt{SF(Basal)}$	TSF^2	

Where TSF is the total schmid factor which is a simple superposition of (SF (Basal), SF (<a> Prism),SF (<a> Prism), SF (2nd order <c+a>), SF (1st order <c> Pyr), SF (1st order <a> Pyr). The function H, is the harmonic mean, for x_1 and x_2 the harmonic mean is represented as follows:

$$H = \frac{2x_1x_2}{x_1 + x_2}$$

3. Min-Max normalization of ALE plots:

Accumulated Local Effects plots in general calculate the local differences between each quantile and the average prediction, this effect is centered around zero, which means that differences can be negative or positive in normal cases. In this work, we have normalized this difference according to a Min-Max normalization:

$$x' = \frac{x - x_{min}}{x_{max} - x_{min}}$$

This step is purely done to understand the relative change that the ALE plot undergoes when changing a specific feature, hence the wording "relative" in our work. Whether this change is negative or positive according to the average is of low importance due to the fact that there is not only accumulated first-order effects, but 2nd and nth order effects that indulging in how they affect the KAM probability prediction would be out of scope of this work.