Applications of Artificial Intelligence in Microstructural Characterization and Optimization of Metallic Materials

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Introduction

Almost every field of research and engineering-including materials science-is being deluged with enormous volumes of data from a wide range of sources (experiments and simulations) at a startling rate. Due to this, the fourth paradigm of research-data-driven science-has emerged. It builds on the enormous data that the first three paradigms of science produced (experiment, theory, and simulation). To examine these data in a way that can contribute to expediting the discovery of new materials and achieving the goals of the Materials Genome Initiative (MGI), advanced approaches for data-driven analytics are required. The fourth paradigm of science makes use of scalable machine learning (ML) and data mining tools to draw conclusions that can be put into practice from such large amounts of data and guide materials design initiatives at various levels (Agrawal & Choudhary, 2019).

Because it enables the simultaneous establishment of a relationship between the structure, method, and qualities, predictive materials modeling has grown in importance as a research area (Agrawal & Choudhary, 2016). Realizing the best material quality is crucial for aerospace applications since the need to use the material for lower fuel consumption, lower process costs, and increased mobility is constant. Crystallographic slip and lattice rotation are two mechanisms that cause the generation of texture and variability in property distributions in such materials during forming processes. Controlling the deformation processes that result in the production of textures with appropriate property distributions is a valuable technique for developing materials (Acar, 2019).

The following sections explain the use of artificial intelligence in materials science with an emphasis on the current studies. The sections have different titles grouped as microstructure recognition, microstructure optimization, and prediction of mechanical properties of metallic materials.

Microstructure Recognition

Elemental composition

ElemNet, a brand-new deep learning network created by Jha et al. (2018), predicts the formation enthalpy of crystalline compounds using just their elemental composition as input. To create the deep learning model, they employed a sizable simulation dataset of DFT computations from the Open Quantum Materials Database (OQMD). The set of 275,759 chemicals and their accompanying formation enthalpies formed the dataset. To test how well a model can function in such a scenario, the authors purposefully did not give the model any domain knowledge. Up to 24 layers, they investigated the fully linked neural network at various depths. Up until layer 17, when the deep learning model

reached a plateau, accuracy increased quickly. Both with and without physical features, ElemNet, the top-performing 17-layer neural network, outperformed conventional machine learning techniques. When utilizing solely elemental compositions as features, the top performing classical ML approach, Random Forest, produced a mean absolute error (MAE) of 0.157 eV/atom and 0.071 eV/atom when using composition-derived physical characteristics as input. ElemNet, which only accepts elemental compositions as input, was found to provide an MAE of 0.055 eV/atom, which is a substantially lower value. ElemNet outperforms Random Forest model (even with physical attributes) for all training set sizes more than 4000, according to modeling studies, which is another example of the superior performance of deep learning models on huge datasets. ElemNet was much faster for prediction time, but it took significantly longer for training.

Crystal structure

A CNN framework for crystal graphics was developed by Xie and Grossman (2017) to learn the properties of materials directly from the bonds between atoms in crystals. In their method, the crystal structure is first displayed as a crystal graph, with nodes representing atoms in a unit cell and edges representing bonds that bind atoms. CNN is then built graphically using convoluted layers, fully connected layers, and grouping layers to automatically extract the best views for modeling the desired properties. Their database contains 46,744 materials with 87 elements, 7 grid systems and 216 spatial groups from the Materials Project (Jain et al., 2013). To predict the formation energy, a simple convolution function with a common weight matrix for each neighboring atom produced an MAE of 0.108 eV / atom. Because they did not consider changes in the strength of interactions between neighbors, they created a new convolution function that does this in the form of a weight training matrix. This led to a significant improvement of the MAE of 0.039 eV/atom. Other DFT calculation parameters in the Materials project received the same structure.

Microstructure characterization

One of the primary procedures to increase our understanding of material is materials characterization, which broadly refers to discovering structural information about a particular material. A proliferation of material image data as a result of advancements in material characterization technologies at various time and length scales, including various types of microscopy, spectroscopy, and macroscopic testing, has inspired the use of deep learning to address this inverse characterization problem (Agrawal & Choudhary, 2019).

Although microstructural characterization is crucial and well acknowledged, classifying it is difficult to undertake. Despite the rapid advancement of digital photography and computer systems, specialists still “manually” assess a given image of a structure to classify its microstructure. In situations where there is a mix of different phases with different substructures, classification can seem incredibly challenging. Any effort in that approach can be beneficial because there is no proof of computer systems that allow the automatic classification of microstructure (Mulewicz et al., 2019).

Microstructure image data can offer a unique perspective on the processes creating microstructures and the mechanisms behind material behavior and performance since they are rich in information about the morphology and suggested a composition of constituent phases. Thus, the study of micrographs (i.e., microstructure image data) is crucial for establishing processing-structure-property correlations and for developing new material systems in numerous materials science investigations. Despite the widespread use of micrographs in material science research, there are still substantial difficulties with reliable and consistent picture data interpretation. These difficulties result from the specialized knowledge and abilities needed to obtain micrographs, the various types of image data

that can be obtained (such as from optical and electron microscopy), the difficulties associated with particular domains for image analysis methods, and more. The use of known AI approaches to microstructure recognition and analysis brings up a possibility for computationally guided experiments and objective, reproducible analysis of picture data as AI (i.e., machine learning) advances in a wide range of domains (Ma et al., 2020).

Development of the model for two microstructural segmentation tasks: i Semantic segmentation of steel micrographs into four regions: intergranular carbides, spherical granule matrix, open grain regions and Widmanstaten cementite. and (ii) segmentation of cementite particles into a spherical particle matrix), DeCost et al. (2019) presents a deep learning solution for the quantitative microstructural analysis of high carbon steels. Because segmentation is a pixel-level operation, as opposed to image classification, a CNN must generate a latent representation of each pixel rather than the entire image. To achieve this, the authors used the PixelNet architecture, in which each pixel is represented by concatenating the representation of each convolutional layer by applying bilinear interpolation to the characteristic inter-pixel map and obtaining a characteristic hypercolumn vector for each pixel. The properties of the hypercolumn pixel are then mapped to the corresponding target or segmentation class using MLP. For the PixelNet convolutional layer, they used a pre-trained VGG16 network and trained the MLP layer from scratch using batch regularization, training, weight loss adjustment and data growth. The basic function of the cross-entropy classification loss and the extension of the focal loss of the cross-classification loss function were investigated using modulation factors and scale parameters to take into account the model reliability and class imbalance, respectively. The data set consisted of 24 micrographs of high carbon steel with a resolution of 645 x 484. Cross-validation was used six times to assess the segmentation accuracy of the model and to compare the actual and predicted particle size distributions and the width of the unclosed region. The segmentation model with concentrated loss functions proved to be the most accurate for spheroid and particle segmentation. Because the model could not recognize particles smaller than 5 pixels in radius, most of the predicted particle size distributions proved to be different from the annotated human micrographs, indicating the need for a high quality input for training. However, their study showed that deep learning is effective for microstructure segmentation and quantitative analysis of complex microstructures with a high level of abstraction. Fig. 1 presents the combined prediction of the microstructure of the particle model and the abstract microstructure model.

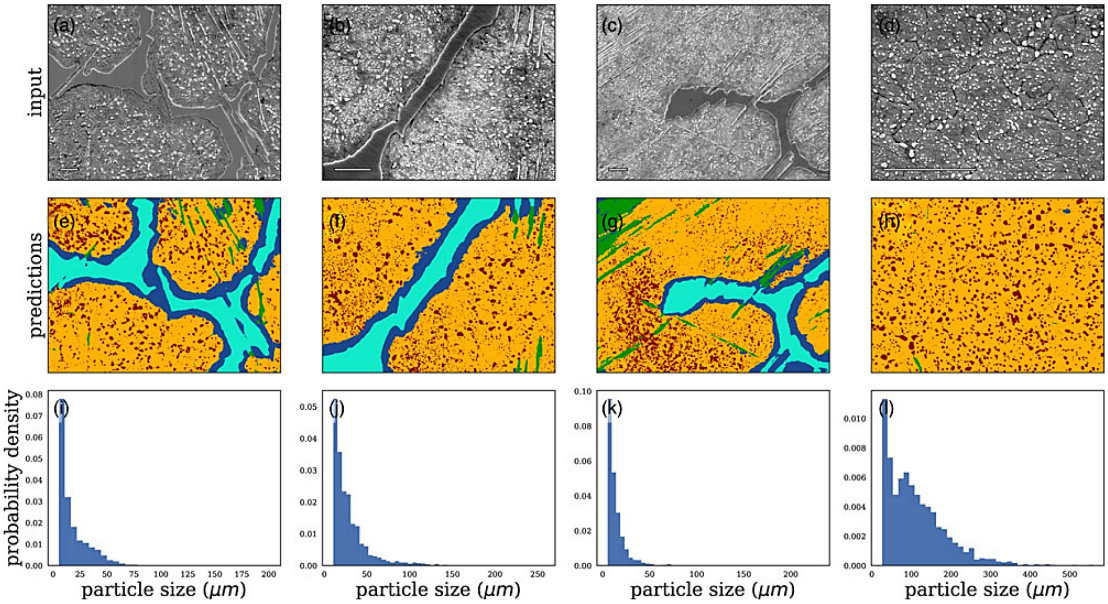

Figure 1. a - d: Micrographs with (e - h) validation set microconstituent predictions and (i - l) derived PSDs obtained by applying the particle segmentation CNN to the semantic microstructure segmentation dataset. Scale bars indicate 10 μm (DeCost et al., 2019)

To categorize steel microstructures, Mulewicz et al. (2019) applied methods from the rapidly evolving field of image analysis based on artificial intelligence, specifically deep learning. The development and application of Deep Convolutional Neural Networks (DCNN) for the categorization of various steel microstructure pictures obtained by light microscopy was the main focus of their research. The neural network was trained using the back-propagation method and the gradient descent optimization technique. Their findings demonstrate that the sophisticated Deep Convolution Neural Network-based system may be used to classify various low alloy steel microstructures.

For automatic microstructure recognition, Chowdhury et al. (2016) used computer vision (CV) and machine learning (ML) techniques. The techniques involved recognizing an important microstructural feature (dendrites) from micrographs that don't have it (just as a human expert would identify that a micro-graph contains dendrites). This challenge of recognition is known as Task 1. Dendrites are a sort of microstructural feature that is not unique to a material system, making Task 1 a high-level microstructure recognition task. It was also accomplished to discriminate between the longitudinal and transverse cross-sectional images of dendritic microstructures (known as Task 2). If Task 1's micrograph was determined to be a dendritic, a second binary classification task was carried out with the intention of differentiating between two distinct cross-sectional views. There were a total of 528 and 188 photos in the data sets for Tasks 1 and 2, respectively. To represent micrographs as feature vectors, approaches for feature extraction and dimensionality reduction were used. Support vector machines (linear and non-linear), voting, nearest neighbor, and random forest models were then used for classification. The classification accuracy for complete and reduced feature vectors, as well as for each feature extraction and selection technique examined, was calculated for each model. Their findings showed that pre-trained neural networks accurately depict micrographs without the need to know the characteristics of the objects or shapes in the images. Additionally, most classifier and feature selection approaches studied showed the highest classification accuracy when pre-trained neural networks were utilized in the feature extraction. Pre-trained neural networks are hence broadly applicable. For Tasks 1 and 2, the highest classification accuracy results were 91.85% + 4.25% and 97.37% + 3.33%, respectively. In a related study, Holm et al. (2020) used convolutional neural network (CNN) layers or feature-based representations to numerically encode the visual information present in a microstructural image, which serves as input to supervised or unsupervised ML algorithms that discover associations and trends in the high-dimensional image representation.

Ma et al. (2020) investigated the representational techniques for microstructures with the goal of using microstructure images to forecast processing conditions. To develop a better machine learning method for picture recognition, characterization, and creating predictive skills tying microstructure to processing conditions, a binary alloy (uranium-molybdenum) developed as a nuclear fuel was researched. They experiment with various microstructure representations and gauge the effectiveness of the models using the F1 score. For differentiating between micrographs corresponding to 10 different thermo-mechanical material processing conditions, an F1 score of 95.1% was attained. The traditional method of using area fractions of different phases was found to be insufficient for differentiating between multiple classes using a relatively small, imbalanced original dataset of 272 images. Instead, they discovered that the newly developed microstructure representation described image data well. Generative adversarial networks were trained to produce artifactual microstructure images to investigate the applicability of generative techniques for enhancing such constrained datasets.

Software for automating metallographic quality control of metals was created by Zhilenkov et al. (2021). It was based on an established approach for identifying the metal grade and on the use of neural networks to recognize photographs of metal microstructures. To ascertain the numerical properties of metals, a neural network's structure has been

devised. They carried out the binarization of the metal microstructure image. Otsu's method was employed for binarization since it is the most successful approach for global binarization. Then, rather than employing the brightness values of objects, the informative elements of the image of the microstructure were created using the properties of the borders, i.e., contours. The Prewitt filter was used to create a precise image of object borders and homogenous region outlines for selecting contours, as shown in Fig. 2.

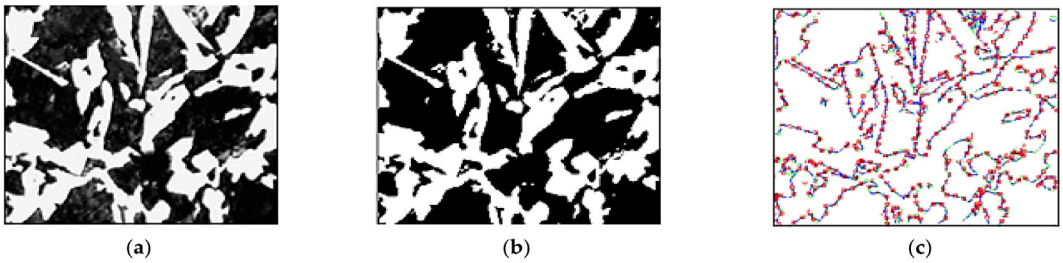

Figure 2. The result of the preliminary processing of the image of the metal microstructure: (a) gray-scale microstructure image; (b) binarization of the metal microstructure image; (c) image thinning operation and boundary detection with Prewitt's filter (Zhilenkov et al., 2021)

The values describing the picture segments of the metal microstructure were established after the base points on the image were fixed and it was vectorized. Triangle hypotenuses, which were created by perpendicular dropped from two neighboring base points, shaped segment elements. The segment elements' sine and cosine values (sin (A), cos (A)) were given into the neural network's input for learning. The Prewitt gradient (Gp), which establishes the contrast value, was also a factor employed as an input parameter. Fig. 3 depicts the design of the neural network used in metallographic analysis to identify the grain point in the metal structure.

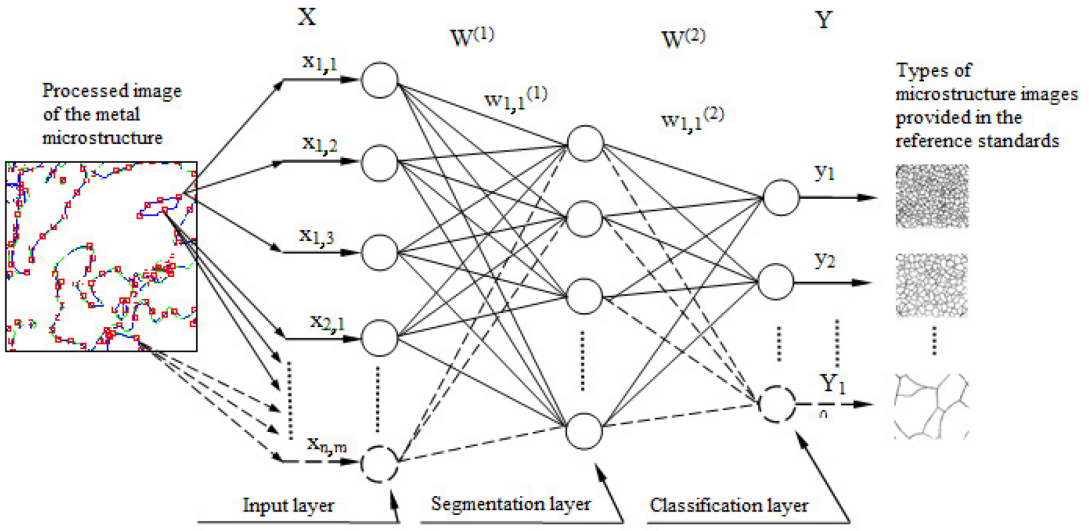

Figure 3. The structure of the neural network for determining the quantitative characteristics of the metal (Zhilenkov et al., 2021)

Microstructure Optimization

The material design groups have recently begun showing a lot of interest in the ML paradigm (Green et al., 2017; Hattrick-Simpers et al., 2016; Mueller et al., 2016; Ramprasad et al., 2017; Ward and Wolverton, 2017). Traditional experiments and computer modeling techniques frequently require a lot of time and resources and are constrained by the experimental settings or theoretical underpinnings, which is the major justification for integrating ML algorithms into material design challenges. As a result, ML has gained

recognition as an effective option for speeding up the process of material discovery and design. To comprehend the nature of the thermomechanical processes and their relationship to the material properties, the process design problem has been investigated in the literature using ML techniques (Abbod et al., 2002; Fang et al., 2009; Han et al., 2011; Zhu et al., 2003).

Acar (2019) used ML techniques to determine the best way to process a texture design. The problem of process design was investigated for this reason by using the transductive learning (TL) algorithm. There are two key data notions in this algorithm. The first one contained "labeled" data, or data that could be matched with a predetermined state (label) from a database of various labels. The second one had "unlabeled" data that could not be directly matched with the labels that were provided, necessitating the use of ML techniques. A database for microstructural textures and deformation processes including tension, compression, xy shear, xz shear, and yz shear was created for this reason. The orientation distribution function (ODF) samples, which represented the starting textures for the various deformation processes, were first created using Latin hypercube sampling (LHS). The final texture information was then stored after simulating the deformation operations. The labeled dataset thus consisted of the known input ODF samples and the related output data. Here, utilizing the coordinate optimization strategy given by the TL method, the goal was to find the labels of the unlabeled designs. The galfenol alloy example problems were addressed using two solutions. In the first application, a previously researched vibration tuning problem's process design challenge (Acar & Sundararaghavan, 2016) was handled for the best numerous ODF solutions.

The findings were verified with the findings of the prior investigation. The TL technique was utilized in the following example to find the ideal deformation process, which could lead to a particularly ideal galfenol microstructure design for a multiphysics problem. Because it provided information on both the ideal and nearly optimal processes, it was discovered that the TL technique was effective to the problem of process design. The best deformation method was then identified using a multiphysics problem's unique optimal galfenol microstructure design developed using the TL methodology. The TL technique was proven to be efficient for the difficulties of process design because it gave information on both the perfect and nearly ideal processes. Any unlabeled ODF information could be used to determine the label (process) using the TL algorithm. For this, LHS was used to create 100 evenly distributed ODF samples for each process (tension, plane strain compression, xy, xz, and yz shear). All processes were predicated on the same process parameters, such as strain rate and total time. Fig. 4 provides a thorough explanation of the TL solution to the process design problem using the TL algorithm, as well as the best ODF solution to the issue. Basic ODF samples were created using LHS in this task, and initial textures were used to simulate various deformation processes. The related deformation processes were recorded and identified on the output textures (ODFs). Using the label data that was previously stored, the label of an unlabeled ODF design was to be found. The coordinate parameter for each label was discovered using the coordinate optimization method. The labels of the unlabeled designs were then assigned in accordance with the criteria for the minimal distance. The optimal deformation process, which was the one most likely to result in the ideal galfenol microstructure design of the optimization problem, was found by solving the process design problem. The best design is the one that minimizes magnetostrictive strain while also meeting the yield stress design limitation (yield stress>555 MPa). Allenol is a magnetostrictive alloy that, in some orientations, exhibits higher magnetostrictive strain values as well as favorable structural characteristics (such stiffness and yield stress). As a result, it is a useful material for applications involving many physics, particularly to enhance the magnetic and structural features that were examined in their study.

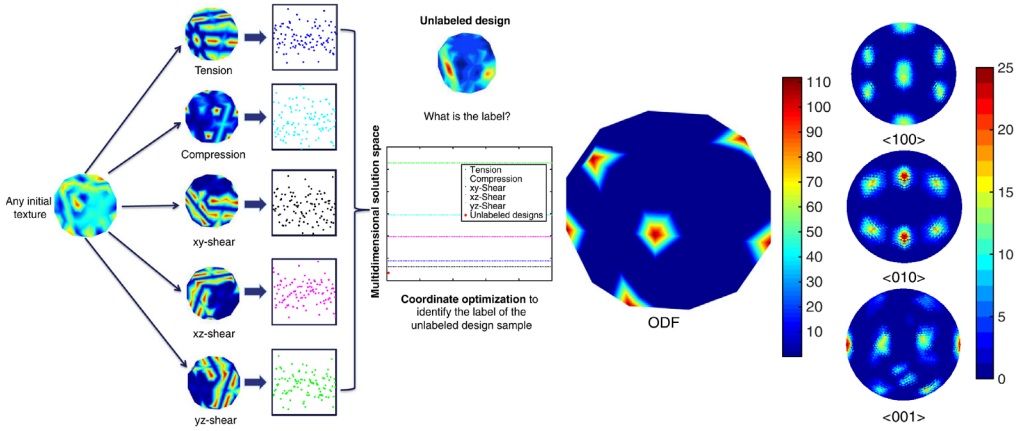

Figure 4. Process design problem of the transductive learning algorithm (left), optimum ODF solution in the problem (right) (Acar, 2019)

Prediction of Mechanical Properties

For the fourth Industrial Revolution's growth of materials science, artificial intelligence has received a lot of attention. Artificial Neural Networks (ANNs), a mathematical technique that matches intricate correlations between input and output layers, can produce superior mechanical qualities with optimal process parameters (Jung et al., 2020). Jung et al. (2020) predicted tensile strength, yield strength and flow ratio using microstructural data of volume fractions using ANNs. They used linear regression and neural network-based algorithms to study combinations of polygonal ferrite (PF), needle ferrite (AF), granular bainite (GB), bainite ferrite (BF) and martensite M (martensite). They calculated the theoretical resistance by calculating the flow limit based on the microstructure. They hypothesized that the yield strength of an alloy could be calculated by simply adding each hardening parameter by work, based on a model governed by a displacement sliding system. The linear regression of the inverse distribution was used to accurately predict the effect of each microstructure on three mechanical parameters. The trend of yield strength deviation with each volume percentage of the microstructure is shown in Fig. 5. (PF, AF, GB, BF and M). The mean absolute percentage errors of the validation and testing set of the deep learning algorithm using hyperparameter matching and cross-validation were 6.59% and 10.78%, respectively. Their algorithm demonstrated good accuracy in predicting experimental data.

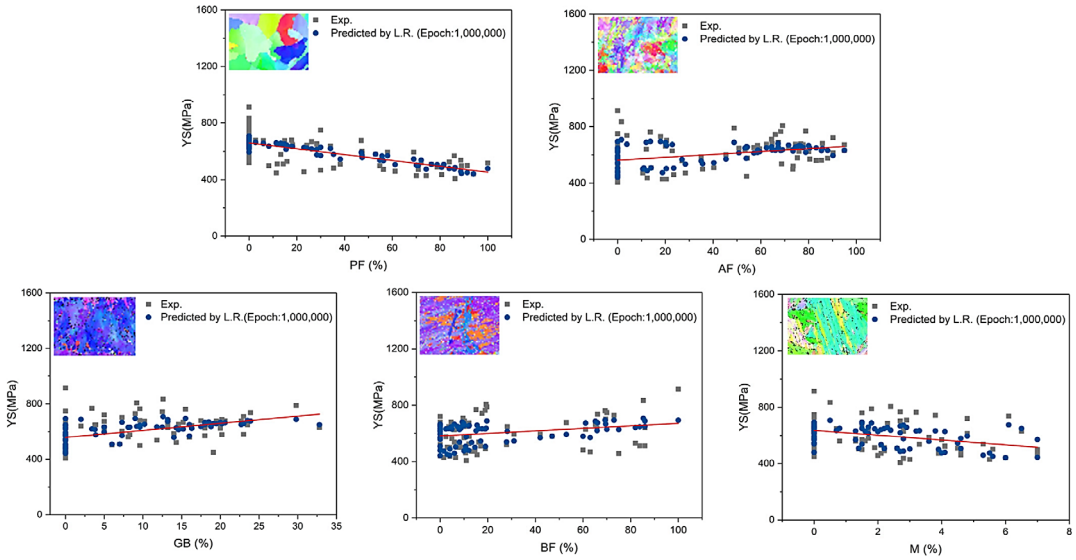

Figure 5. Yield strength tendency prediction with PF, AF, GB, BF, and M via back propagated linear regression (Jung et al., 2020)

In modeling the relationship between the chemical composition and properties of DP steels, Krajewski and Nowacki (2014) suggested a method for determining the tensile strength and yield strength of dual phase (DP) steels using ANNs. Based on the literature sources, they gathered a material database outlining the characteristics of the DP steels. To calculate the impact of alloying components, heat treatment settings, transition temperature, and microstructural characteristics on the mechanical properties of steels, an ANN model was developed. The BFGS (Broyden-Fletcher-Goldfarb-Shanno) training algorithm was used to create the chemical makeup of DP steels that would have the necessary tensile strength. The logistic activation function was utilized to forecast using the MLP 14-7-2 multilayer feed forward neural network (14 inputs, 7 neurons in the hidden layer, and 2 outputs: yield strength and tensile strength). Using a neural network simulation, Fig. 6 depicts the effects of two sample alloying components, including carbon, silicon, and manganese, on the tensile strength of steel under set heat treatment conditions and constant concentrations of the other alloying elements.

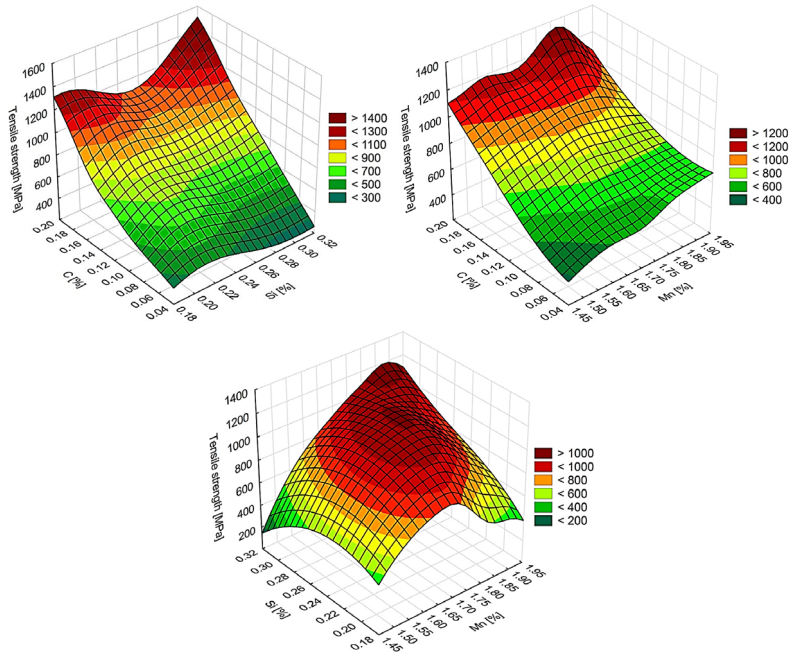

Figure 6. Effect of the concentration of alloying elements on the tensile strength of DP steels; carbon and silicon (left), manganese and carbon (middle), manganese and silicon (right) (Krajewski & Nowacki, 2014)

Li et al. (2021) used machine learning to predict the hole expansion capacity of high strength steels using an experimental dataset made up of the phase constituents of 55 microstructures and corresponding properties, such as yield strength and hole expansion capacity, that were gathered from the literature. These data were statistically analyzed with an emphasis on the hole growth capacity with respect to individual phases, phase combinations, and the total number of phases. The prediction of hole expansion capacity based on phase fractions and chemical composition used various ML techniques. Based on phase fractions and chemical composition, deep learning produced the hole expansion capacity predictions with the highest degree of accuracy.

The Materials Genome Integration System Phase and Property Analysis (MIPHA), an ML tool, was created by Wang et al. (2019) for inverse analysis of steels, where a genetic algorithm was used to explore the potential best-balanced property of tensile strength and total elongation and its corresponding microstructure and processing conditions. The analytical model was fitted using a standard ANN with one hidden layer and the sigmoid function as the activation function. According to their findings, the properties-to-micro-

structure/processing analysis approach was successful in identifying the model that produced the greatest outcomes, had the best property balance, and had the most plausible correlations between processing, microstructure, and properties. It has been discovered that a microstructure-comprising Widmanstatten ferrite, bainite, and martensite is advantageous for a good balanced property.

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