Application of Machine Learning in Determining the Mechanical Properties of Materials

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1 Introduction

As per the national research councils of India material characterization should describe feature such as structure of material, composition, defects, etc. with application. Material characterization involves chemical, physical and mechanical properties which describe the material in best manner. To understand the physics of engineering material under the action of external forces (which may be of contact and non-contact type) is known as mechanical characterization of material. These mechanical properties play an important role in characterization of material which helps the research to find its correct application. Evaluation of mechanical properties relies on experimental data [1] obtained from distractive and non-distractive testing. And mathematical model (based on governing law) which interpretiate the mechanical properties from data obtained from experiment. Increasing demand of the society result in discovering of new material having superior properties with vast range of application are been required. Evaluation in material science field can be best described into four phases or paradigms [2]. First phase start from stone-age past back to thousands of years where by only metallurgical observation help in predicting

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the characteristic of material, this is purely empirical. Second phase start near about sixteenth century where scientists have developed mathematical models to correlate the physical relations. In these paradigms conventional laws have been formulated in the form of mathematical equation. But with time the complexity of developed mathematical model become too complex, result in raising question on the solution obtain from the above analytical methods. In the mid of nineteenth century, advancements in computational science increased that gave rise to the third phase. Any mechanical properties of the material cannot be best described by only one mathematical model or conventional law; there may be several concept which may describe the single property in best way. Therefore experimental data is been required which is been interpreted through mathematical models with the help of computational science. Molecular dynamic and density function theory are been some of the examples in material science in this paradigm. Data generated from experiment and simulation from computer give rise to fourth phase where calculation of mechanical properties is based on large set of data also known as data driven paradigm [3]. Large data set obtained from different experiments including structure patterns help in determining the hidden correlation which were not visible in small data sets result in horizon of twenty-first century research. Figure 1 represents the four paradigms of material science starting from stone-age to twenty-first century.

2 Big-Data

To meet the specific requirement of industries or scientist discovery of novel material or unknown properties of known materials is been evaluated on the basic of data obtained from different source which may or may not relate the property in theoretical concepts. But contain some hidden correlation that may describe the behavior of the material and the huge amount of data obtained from different source comes under big-data. Big-data is been characterized by five-V models i.e. *volume*: concern about the size of the data, *velocity*: data generation speed, *variety*: diversity of data generated, *veracity*: quality and accuracy of data generated and *value*: value provided the data generated [4, 5]. Development in sensors helps in collection of data, but bigness of data have their own challenges such as storage, visualization, analysis, and retrieval. Suppose data obtained from heterogeneous sources (from different experiments) have the problem of correlation in between them, inconsistencies within it, some missing value, reliability issue, etc. These are the major challenges comes in the path of scientist while working in the field of material science. In the field of computational material science, European center of excellence, Novel Material discovery (NOMAD) having concept "FAIR" of big-data i.e. **F**indable for anyone interest, easily **A**ccessible, standard representation which make it **I**nteroperable and **R**eusable [6]. Different stages involve in mechanical characterization of material are and also shown in Fig. 2, data obtained from the heterogeneous source may first pre-process to identify the correlation of in between the data; after that identification of key feature/factor which may help in data reduction/selection; after that mathematical

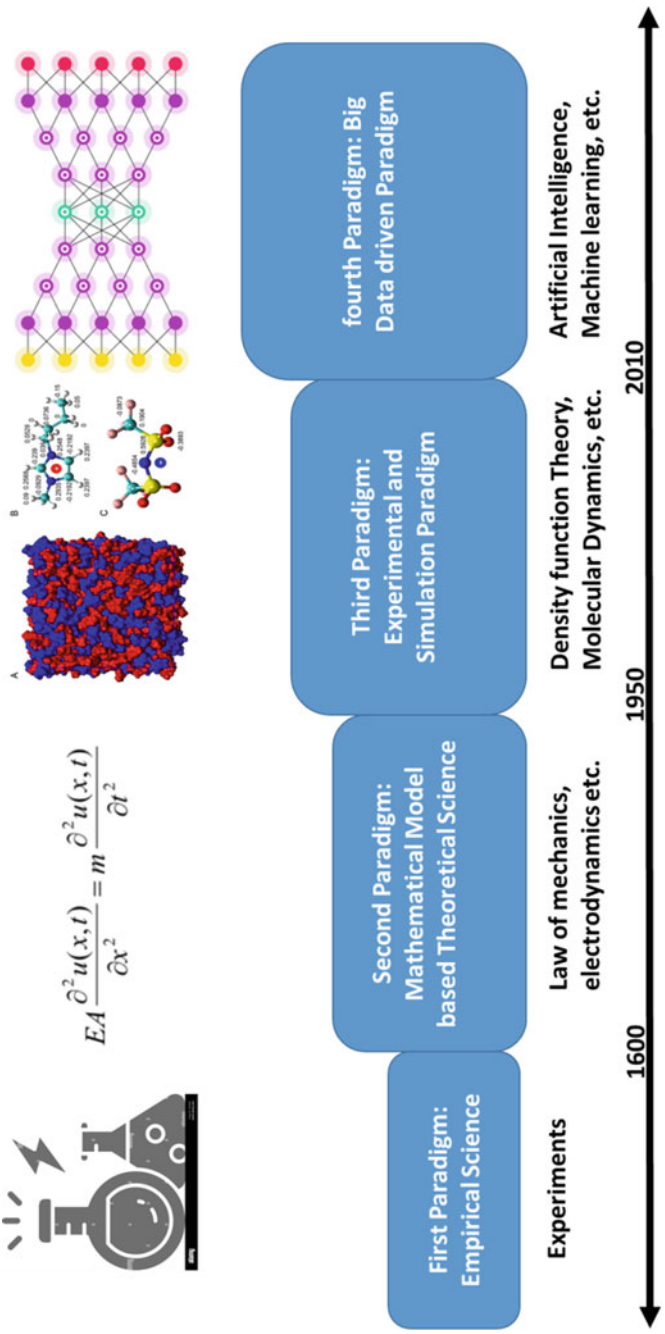

Fig. 1 Four paradigms of material science starting from stone-age to twenty-first century

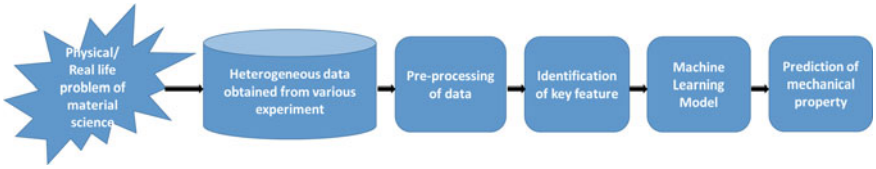

Fig. 2 Different stages involve in mechanical characterization of material

model based on machine learning is applied on the data; finally this machine learning model will predict the mechanical property on the basic of data provided to the model. At last predicted value of mechanical property is been validated. Therefore after big-data computer intelligence plays an important role where machine learning comes into picture.

3 Machine Learning

Machine learning (ML) should be describe as generating computer intelligence with the help of algorithm which perform certain task on the given relevant data [7]. Next paradigm in the field of material science is application of artificial intelligence and machine learning [8–10]. Increase in computational power help the scientific community to involve lab automation, parallel experiments and effective experiment design also known as high throughput experimentation (HTE). Through HTE correlation in processing, microstructure and composition of material [8–11] is been possible. ML models are broadly classified into four categories: (1) Supervised Learning: In this type of model labeled data is used to train the model and predicts the outcome [12]. Some supervised learning algorithms are neural networking, linear regression, Naive Bayes, etc. (2) Unsupervised learning: In this type of model unlabeled data is used to train the model, clustering of data is done and the outcome is been predicted. Some unsupervised learning algorithms are k-nearest neighbors, k-mean clustering, etc. (3) Semi-supervised learning: In this type of model some data is labeled data and some is unlabeled [13]. (4) Reinforced learning: this model is based on reward and penalty approach [14]. ML has wide application in every area of science and day to day activities such as communication, transportation, medical, business, material science, social media, and industrial research [15]. In the field of material science ML is used to predict new stable materials [16–18], predicting of material properties [19–21], inorganic chemistry [22–24], predicting properties of material [25–27], analyzing complex reaction [28], understanding crystal structure [29], guide experimental design [30], etc. In this chapter a brief review of application of machine learning in the field of determining the mechanical properties such as tensile strength, fatigue behavior, visco-elastic study, and etc. have be done.

4 Tensile Strength

Characterization of material is done through determining the mechanical properties such as tensile strength, yield strength, % elongation, etc. It is the behavior of material under the action of external forces. Mechanical properties of material depend upon many factors such as microstructure, alloying composition, fabrication processing parameters, and other external factors. As per present scenario most of the researcher employ the universal testing machine to determine the mechanical properties of material. But there is no mathematical model where all the above governing factors will be include, therefore the role of machine learning comes into picture. Wang et al. [31] applied the machine learning algorithm to determine the elongation and yield strength of reduce activation ferritic/martensitic steels (RAFM). To perform the ML algorithm database is been developed through experiments. And to maintain dimensional equality normalization was performed as preprocessing method for feature engineering. About 80% database is been used to train the ML model and 20% to test. Initially there are about 19 feature, after artificial selection 8 feature (due to narrow data range following were content Ni, Nb, V, Mn, Mo, neglected; due to testing accuracy following were neglected content of P, S; and due to small dataset of time, temperature of austenitizing is been neglected) were ignored. Random forests model was employed as ML algorithm to find out the impact of remaining 11 features (content of C, Cr, W, Si, V, Ta, Ti, N, B, Temp., and Time) on yield strength and elongation of RAFM. Moreover, last-place elimination rule was also been employed to eliminate the feature which less correlate. Results show that tempering temperature, content of C and tempering time show the highest correlation in predicting the yield strength of RAFM followed by content of Cr, Ti, W and B. Outcomes of ML model shows similarity with RAFM steels principle of physical metallurgy i.e. formation of MX carbonitride during tempering process of RAFM steel play an important role in strengthening mechanism [32].

Sasikumar et al. [33] predict the ultimate tensile strength of epoxy/unidirectional carbon composites using back propagation algorithm based on Artificial Neural Network (ANN). Acoustic Emission (AE) response of epoxy/unidirectional carbon fiber is been recorded, AE sensors were placed on both side of the specimen. Total of about 18 dataset were generated and three mode of failures were studied i.e. (1) fiber breakage: since most of the load is taken up by the fiber, therefore highest energy and amplitude is been generated, (2) delamination (in case of unidirectional fiber splitting of fiber): duration of this mode is short and amplitude and energy is also lesser than fiber breakage failure and (3) matrix cracking: this failure occurs throughout the test. AE characteristic produce were recorded for each failure mode i.e. AE hits and ultimate tensile strength. Three layers ANN model were used to fit the data obtained with 45 neurons at middle layer, Levenberg-Marguart algorithm employed with linear transfer function. Results show about 9.5% error which makes ANN more provident method to predict the tensile strength using AE emission.

Santos et al. [34] apply machine learning approach to predict the mechanical properties with foundry process parameter. 25 variable parameters were taken into account for 889 casting datasets. About 10 different ML classifiers such as Bayes TAN, Bayes Hill Climber, Bayes K2, Naive Bayes, KNN algorithms were used. Results show that Hill Climbing classifier give best result for lower training datasets whereas in case other classifier their accuracy increases with increase in training dataset.

Sterjovski et al. [35] apply the artificial neural networks to predict the mechanical properties of steels. Focus of the work is on to predict the impact strength of quenched and tempered pressure vessel steel exposed to multiple postweld heat treatment cycles on the basic of alloy content and heat treatment processing parameter (Model 1); hardness of the simulated heat affected zone of weldment in pipeline and tap fitting steels after in service welding on the basic of alloy contents and cooling time (Model 2); and the hot ductility and hot strength of various micro alloyed steels over the temperature range for strand or slab straightening in the continuous casting process on the basic of treatment conditions and chemical composition (Model 3). ANNs model variables is classified into material characteristics (composition of alloying element, such as %C, %Mn, %Cr, etc., thickness and hardness) and processing parameters (temperature, cooling rate, time, etc.). For Model 1 10 input variable i.e. cooling type, time, thickness, orientation, temperature, content of C, Cr, Mn, and B were studied. In Model 2 16 parameters were taken and 9 were taken for Mode 3. For all the models content of carbon play a significant impact. For Model 1 holding time and temperature play important role, impact strength decreases with PWHT time. In Model 2 with decrease in cooling rate from 150 to 30 °C/s result in drop in hardness. For Mode 3 with increase in test temperature hot tensile strength decreases.

Datta et al. [36] apply the concept of neural networks and genetic algorithms in designing multiphase steel for balanced strength and ductility. Major challenges in multiphase steel to use the optimum amount of alloying elements such that it has maximum strength without compromising the ductility. Moreover, thermo-mechanical controlled processing parameters such as cooling rate, rolling temperature, reheating temperature and deformation in rolling stages also play an important role. For modeling of neural networking thermo-mechanical controlled processing parameters and alloy composition were taken as input variable and yield strength, elongation and tensile strength as output parameter. Further to reduce the neural network connectivity two methods were employed. First is intuitive pruning algorithm [37] which is used to remove the lesser significant connections. In second approach genetic algorithm [38, 39] (predator prey algorithm and pareto front is employed to minimize the training error). Results show that rolling temperature does not play any significant role in predicting the yield strength and ultimate tensile strength of multiphase steel. Reason regarding that conclusion is that rolling temperature is maintain higher that the recrystallization temperature therefore amount of dislocation during rolling is lesser due to which alteration in yield strength and ultimate tensile strength is insignificant. Major factor which influence the multiphase steel are precipitation hardening and post rolling cooling rate. Results show that carbide forming elements have less effect as compare to Cu (strain hardening) in

case ultimate tensile strength. Whereas cooling rate after rolling play important role in microstructure construction and found to most significant input variable even for percentage elongation also.

Zhang et al. [40] applied the deep learning concept for elasticity imaging of non-homogeneous material through Physics-Informed Neural Networks (PINNs) on the basic of which diseased and normal tissue cab be identified. Accomplishment of objective was done using two neural network one for solution approximation and other for unknown material estimation. The objective is to determine the material properties by observing displacement data for plain strain problems for incompressible Neo-Hookean hyper-elastic materials. Formulation loss function involves displacement data, physics information of partial differential equation, boundary condition and incompressibility constraint.

Matzbower et al. [41] applied the concept of neural networking to approximate the ductility and strength of welding shipbuilding steel alloys. Database of 189 weld steel alloys samples were been generated which include chemical composition (such as content of C, Mn, Si, Cr, Ni, Mo, Cu, S, P etc.), elongation and cross-section area reduction and weld cooling rate as an input variable and ultimate tensile strength and yield strength as output variable. All input variable were been normalized within the range of $\pm$ 0.5. About 80 neural models were created with varied number of hidden units and 5 random initial seed set. The output y is the linear function of bias and hyperbolic tangent transfer function. Results show that about ¼ dataset doesn't satisfied the model in case yield strength. Noteworthy input variable which had significant impact on yield strength are content of Mn, C, Ni, Ti, Mo and cooling rate.

Shigemori et al. [42] applied the concept of Just-In-Time (JIT) methodology to developed quality design system for steel. Focus of the work is to decide the best manufacturing procedure as per the desire quality target for steel bar. Initially the production of steel slabs is done by altering the chemical composition. To obtained desire shape and size cold working (rolling process) of the steel slab heated to specific temperature is done. Desirable mechanical properties and microstructure is been obtained through cooling process which may further be temper rolled and heat treated to again modified the properties. In this work quality index of the steel or output parameter taken were tensile strength, yield strength, toughness and elongation. And on the other hand alloying element content, cooling process, rolling process and extraction temperature were taken as input parameter for mathematical model. Mathematical model is based on locally weighted regression approach type of JIT modeling which can be employed for nonlinear processes. Quality designing system consists of three models first one to select the initial input values so that value of initial objective function (it is deviation of product quality from target value) is minimum; second one for locally weighted regression models which generate nonlinear relation between quality and manufacturing condition, and third module is for deriving the optimal manufacturing conditions by employing quadratic programing methods. Results show that accuracy of locally weighted regression is higher as compared linear regression.

Swaddiwudhipong et al. [43] employed the least square support vector machines to characterize the aluminum alloys (Al6061 and Al7075). Previously many researcher had used reverse analysis through iterative process but due to high nonlinear nature make it complex. Other approach is to use analytical model developed between load-indentation parameters and material properties. Latter on concept of artificial neural networking is also been adopted by the researchers [44, 45] for material characterization when single indenter is been used to extract the data for thin films, which further extended to elasto-plastic materials [46]. In present work validated results obtained from FEA (using ABAQUS software) of indentation tests using conical indentor based on large strain and deformation model were taken as input in least square support vector machines (LS-SVM). The four LS-SVM models were developed using MATLAB 6.5 based on structural risk minimization principle. Problems like over fitting and large deviation are overcome by regularization and final unction is obtained with incorporation of regularization and loss function. Outcome shows that LS-SVM model gives more accurate result of Young's modulus and yield strength rather than position's ration.

5 Fatigue and Creep

Behavior of material under the action of cyclic loading is known as fatigue. Fatigue behavior/characteristic of material is determined by calculating the no. of cycles before failure also known as fatigue life. Abdalla and Hawileh [47] employed radial basis function (RBF) ANN for modelling and simulation of fatigue life (low-cycle fatigue life) of steel bar. For training the ANN model input parameters were maximum tensile strain (sinusoidal axial strain with 0.05 Hz frequency ranging from 3 to 10% beyond yield point) and strain ratio ($-1, -0.75, -0.5, -0.25$ and 0). And no. of cycles to fail the material is been evaluated through fatigue test taken as output parameter which is been evaluated by Coffin-Manson equation [48–50]. ANN model is based on back-propagation feed forward with random selection of initial weight values. ANN model consist of two additional hidden layers with four neurons in each layer. First hidden layer consist of Gaussian activation function while one output layer and two additional hidden layers consist of tangent hyperbolic activation function. Accuracy of ANN model is high with the normalized square error 0.0428 and R value 0.9869.

Application ANN also been used predict the failure life of composites material now a days. Lee et al. [51] predict the fatigue life of the carbon and glass fiber reinforced epoxy composites using ANN method. Object of the work is to develop the model for predicting the fatigue life for newly developed/existing material having lesser fatigue testing results. Only approach available is developed mathematical model using physical laws by evaluating material properties and damage at microstructure which is time consuming and yet satisfactory result is also not obtained. Dataset is been obtained by fatigue testing of material with R rations 0.1–0.5. Three input parameters were taken i.e. are stress ratio, stress range and mean

stress and on the other hand fatigue life was taken as output parameters. ANN model prediction give good result for median life as compared to minimum failure life.

Agarwal et al. [52] determine the fatigue strength of steel based on composition and processing parameter by employing different data science techniques such as ANN, decision trees and regression. Database is been obtained from MatNavi (National Institute of Material Science) which is world largest database developed at Japan. Database consists of low alloy steels, spring steels and carburizing steels having 25 input variable parameters having following classifications: (1) Chemical content such as weight percentage of different alloying element C, Si, Mn, S, Ni, Cr, Mo, Cu, etc.; (2) Upstream processing parameters i.e. reduction ratio, ingot size, non-metallic inclusions, etc.; (3) Heat treatment parameters such as time, temperature, and processing conditions for different process, and; (4) Mechanical properties such as yield strength, ultimate tensile strength, %elongation, hardness, fatigue strength, impact value, etc. Preprocessing of database is done for feature selection and R, WEKA and MATLAB were used as data processing software. Result shows that tempering time, Carburization temperature and Diffusion temperature have the highest correlation with fatigue strength. About 12 different ML models were used out of which MPR and M5 model tress show the best result with R^2 value of 0.98.

Zhang et al. [53] applied the concepts of genetic algorithm and support vector machine (SVM) to determine the fatigue life of material. SVM machine learning technique is applied when the database contain smaller sample with good accuracy result. In this technique nonlinear mapping of input variable into infinite-dimension space by creating hyper plane which classify the database into classes. Kernel function (Gauss function) was also been incorporated to solve nonlinear problem through SVM. Purpose for introducing the kernel function is to overcome the dimensionality problem, help in nonlinear transformation expressions and provide different mapping space having different properties. Accuracy of SVM depends upon the three factors: Penalty factor, higher is the value higher is the fitting but time consuming also even too high value result in over-fitting; Lower fitting accuracy, higher is value lower the no. of support vectors result is reduction in the complexity of the accuracy of model; γ, smaller is the value, poor performance of radial based function and vice versa but too high value may cause poor generalization ability. Genetic algorithm approach was employed to optimize the parameters as parameter selection is one of the major problem where theoretical guidance cannot help. SVM model was used to predict the P91 steel base metal and welding consumable taken from literature of Ji [54]. Holding time is taken as input parameter whereas fatigue life as output parameter. Genetic algorithm-SVR shows the highest accuracy with R2 of 0.99 on training sample. The authors have a vast experience in the field of molecular dynamics and experimental characterization of composites materials [55–106].

6 Conclusion

This chapter shows the various machine learning techniques applied by different researchers towards characterization of mechanical properties of material. These articles review literature on the application of machine learning in the field of fatigue failure, creep-recovery behavior of material, tensile strength, etc. Utilization of machine learning techniques in the field of material characterization is growing day by day. ML has a vast future in the field of material characterization which is not only limited to above characterization techniques.

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Conflicts of Interest "There are no conflicts of interest to declare by the authors."

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