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Research Network Analysis and Machine Learning Modeling on Heusler Alloys

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Abstract

Heusler alloys are an incredible class of inter-metallic materials with different compositions and over 1500 members. Though discovered a century back, they are an active area of physics and material science research. Novel properties and potential fields of applications materialize constantly. Even the alloy system is extensively investigated owing to its shape memory behavior and prospective relevance in the development of actuator devices, where strains are controlled by applying an external magnetic field. Heusler alloys are currently the material of interest due to their properties leading to their use as shape memory alloys and topological insulators. Hence, predicting and determining their composition and structure is imperative before synthesis. Utilizing the conventional method in determining the possible changes in the properties and the structure of the proposed compositions is tedious and time-consuming. In the current consumerism-driven environment, we require a faster method to predict the structure of the proposed alloy or compound or other parameters for the desired application. Once the prediction is made, it must be tested experimentally by synthesizing the material and characterizing its behavior. This analysis is focusing on network analysis with a supervised machine learning approach to study the properties of Heusler alloys with their application as shape memory alloys.

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1. Introduction

Fritz Heusler discovered a unique alloy with the composition Cu_2MnAl in 1903, which marked the beginning of a new era in the world of material sciences. It was observed that this alloy behaved like a ferromagnet, despite its constituent elements being nonmagnetic.[1] This seems to be an exemplary finding as it paved the way for promising development in the field of magnetism,[2] and now they are a family of thousands of such compounds, including the copper-manganese-based alloys containing elements like bismuth, boron, arsenic, tin, aluminum, *etc*. which were named 'Heusler Alloys.' The presence of Mn has been known to lend the magnetic moment to these alloys. Interestingly with the count of valence electrons, different properties of Heusler compounds can be determined.[1,3] Heusler compounds were recognized as intermetallic compounds because of their beautiful yet peculiar atomic order. The general stoichiometry is in which two transition metals and one main group of elements are combined to form Heusler alloys of type X_2YZ (full Heusler) or XYZ (half Heusler) with an L21 crystal structure.[4] Sometimes, Y may be replaced by a rare-earth or alkaline element.[5,6] Most of these alloys are either Cobalt (Co-based) or Nickel (Ni-based). Generally, for a ferromagnetic alloy, every element in the compound ought to contribute to the magnetic dipole moment.[1,3,4] But a typical Heusler alloy comprises mainly nonmagnetic materials that give rise to a magnetic moment when alloyed together. Heusler alloys are in demand amongst magnetic nanoparticles due to their considerable spin polarization and half-metallic nature.[7] This spin polarization factor is 100% at the Fermi surface of the material. The most remarkable aspect that enhances the half-metallicity of ferromagnets is that these compounds have the dual behavior of a semiconductor for one of the spin channels at its Fermi surface and metal for the second spin channel.[8] X_2YZ compounds are primarily responsible for magnetic properties, including multifunctional properties like magnetocaloric, magneto-optical, and magneto-structural characteristics. In this technologically progressed era, Heusler

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alloys are emerged as prominent materials in the research fields, including spintronics,[9] ferromagnetic shape memory alloys,[10] thermoelectric,[6,11] data storage devices[12] and topological insulators.[13] These applications result from their unique thermodynamic, magnetic, and electric properties and versatility brought about by modifications in solvent and solute concentrations. While coming to practical applications, thin film technology is mainly studied using Heusler compounds because these two-dimensional materials are in the nanometer range.[14,15] Further, when the length scale is confined to three-dimensional, the resultant lead to Heusler nanoparticles exhibiting size-dependent physical and structural properties, which are of supreme significance not just in basic scientific interests but also for future applications.[11,16] Compared to the research on magnetic nanoparticles, ferromagnetic Heusler nanoparticles have a sprouting prospect. Amongst these, Co-based and Ni-based HAs have attracted excessive interest because of their magnetic properties, high Curie temperature, and high saturation magnetization.[7,17-20] Current developments in Heusler alloys illustrate phase transformations with changes in lattice factors and near-transition temperature ferromagnetic ordering.[21,22]

In this paper, state-of-the-art has been carried out to study the properties of bulk and nano Heusler alloy. Additionally, Machine Learning algorithms were used to predict the multifunctional properties of the numerous compositions of Heusler alloys. The meta-review consists of the methodology with which the papers were analyzed, and the data collection based on specified keywords followed by the ongoing research in the Heusler alloys depending upon their disciplines and the topographical areas. Extensive network analysis has been done by correlating diverse statistics such as the journal, author, year, territory, funding agencies, and citations. Along with these, a machine learning model was also incorporated for designing the parameters that influence the multifunctional property, such as the shape memory application of Heusler compounds. The proposition of this investigation has made us realize the potential of application-oriented studies to be done on Heusler compounds by studying their structural, electrical, and magnetic properties which is mandatory for further developing the material for any multifunctional applications like memory and storage devices as well as shape memory applications.

2. Few interesting findings on Heusler alloys by different research groups

The breakthrough research was done by Dr. Claudia Felser, a full-time professor and the Director and Scientific Member at Max Planck Institute for Chemical Physics of solids in Dresden for research in advanced Sciences. Their group has published the work in the journals like Nature and Science in the field of experimental and theoretical condensed matter Physics as well as in Materials Science. A remarkable discovery by her group in 2006 was a high magnetic moment and Curie temperature of about 6μB and 1100K for a half-metallic ferromagnet. The class of Heusler compounds was published in the peer-reviewed journal of Applied Physical Letters, and the year 2013 witnessed a noteworthy finding on inverse Heusler compound Mn_2CoAl because Mn is a very tricky metal that has various oxidation states and hence the theoretical studies on its spin numerous research groups did gapless magnetic semiconducting behavior. Here her group has proved the first experimental verification of this study. The finding was below room temperature, *i.e.*, less than 300K; the compound showed temperature-independent properties such as lower carrier concentration and less conductivity leading to an almost vanishing See beck coefficient. The review article called "Simple rules for the understanding of Heusler compounds," authored by Dr. Tanja Graf, Dr. Claudia Felser, and Dr. Stuart S.P. Parkin, is the highly cited and the most useful for the research community working in the domain of theoretical or experimental aspects of Heusler compounds as the article contains immense information on and has got published in Progress in Solid State Chemistry, published by Elsevier in the year 2011 and is available online. The article reviews the properties of Heusler compounds like magnetocaloric, magneto-optic, magnetoelectronic, and magneto-transport properties as the combination of exceptional transport properties with magnetism is a great amalgamated study for various applications, including shape memory materials, thermoelectric materials, spintronics, superconductors, and topological insulators. Fig. 1 represents the interconnection of Dr. Claudia Felser's achievements, research positions, memberships, and active research on our topic of interest. She and her research associates have pioneered the prediction and discovery of engineered quantum materials. There has been an immense amount of research done by diverse groups. Some significant ones were mentioned, like works on Co_2MnSi and Co_2MnGe using ab-initio computations, indicating that they show half-metallic characteristics.[2,23] Studies were done on Co_2MnGe alloys and observed the magnetoresistance and showed ferromagnetic behavior with a high Curie temperature.[24] The magnetocaloric effect was observed in magnetic tunnel junctions created in Co_2MnSi.[25,26] Large magnetoresistance was observed in magnetic tunnel junctions due to creating magnetic passage intersections utilizing Co_2MnSi as one magnetic cathode and $Co_{75}Fe_{25}$ as a magnetic anode.[2] Dong *et al.* late figured out how to pass spin-polarized current from Co_2MnGe into a semiconducting structure.[27] Studies were done to know the impact of substituting Fe for Mn in Co_2MnSi films and have indicated that the magnetic spin moments are feasible with the amount of doping.[28] Barocaloric effects were studied on MnNiSb as it showed large entropy change and martensitic transition by inducing a magnetic field.[29] The electronic structure and band structure calculations of $Co_2CrFeAl$ were concluded with high magneto crystalline anisotropy energy and magnetization in the martensite phase.[30] The half-metallic ferromagnetism in Co_2TiAl and

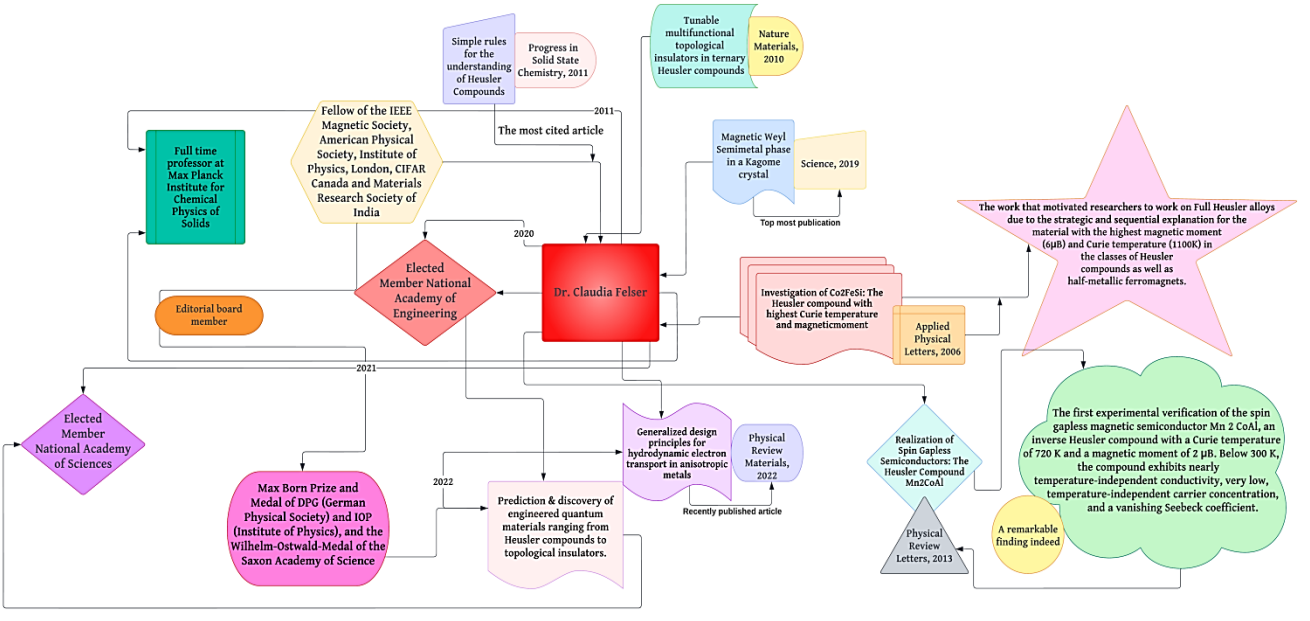

Fig. 1 The chart represents the topmost research group working on Heusler Alloys for different potential applications.

Co_2FeSn studied that high thermoelectric performance leads to less thermal conductivity.[31-33] The unique route developed for developing CFA nanowires through the electrospinning method, which seems to be the most versatile process for fabrication in nanotechnology and is capable of forming various fiber assemblies, thus, enhancing the performance of nanofibers and permitting application-based specific modifications.[34]

3. Selection of research articles with exclusion-inclusion criteria for network analysis

Experimental synthesis of Heusler alloys is the beginning part of every research articles. The state-of-art of research has mostly focused on the experimentation, instrumentation and computational studies on various aspects of Heusler alloys ranging from their tunability in magnetic properties and multifunctional behavior and its functionality range from thermoelectric, spintronics, shape-memory, topological insulators, *etc*. The research articles published by studying these properties were done through modifying the synthesis techniques from bulk to nano, *i.e.*, from preparing ingots under high vacuum arc melting, induction melting, thin films through sputtering, laser ablation, electrodeposition, nanoparticles through ball milling, thermal decomposition, electrospinning *etc*. Hence, it's necessary to validate experimentally along with the theoretical studies made through certain approximations like first principle calculations through the art of density functional theory. Hence there is a need of comprehensive metric analysis to be carried out to determine the uniqueness of literature, influential research, and prominent researchers in the advancement of Heusler alloys through geographical attention to the research carried out, statistics of the author's affiliation, contributions of the author, details of the journals where papers have been published and their statistics, as well as an analysis of citations. The categorization as per subject area were done and most research is carried out in physics with prominent results getting published in theoretical and experimental physics, followed by material science. In engineering, along with science and technology, excluding basic sciences, this idea of Heusler alloys and the quantity of research being carried out constitutes very less. In the field of chemistry, including biochemistry and electrochemistry, there is less research on Heusler alloys than in material science. The crystallography area contributes highly toward the study based on Heusler alloys as the structure determination is an important aspect in furthering the studies. It is also evident that a significantly less amount of research has been carried out in niche areas of Machine Learning and Artificial Intelligence. The Fig. 2. represents the overview of the literature data attributes preferred over six different databases like, Scopus, Web of Science, Science-Direct, SCImago, Google Scholar and Clarivate. The keywords were categorized as master which is the main keyword of research, *i.e.*, the Heusler Alloys and primary which are the subsequent research areas on which Heusler alloys are of wide importance. These were chosen according to the different permutation and combinations of the keywords and the relevant hits were selected. Among them, 129 research articles were selected by filtering it out with inclusion criteria such as highly cited, full-length papers that are available to download, journals that published experimental and theoretical observations. Additionally, the articles focused only on the core journals in the field of physics and chemistry. Book chapters and conference proceedings were excluded. Even the duplicates were discarded as same keywords were used in different data sets. Finally, a dataset was prepared with an access to 123 research articles and that were utilized for network analysis.

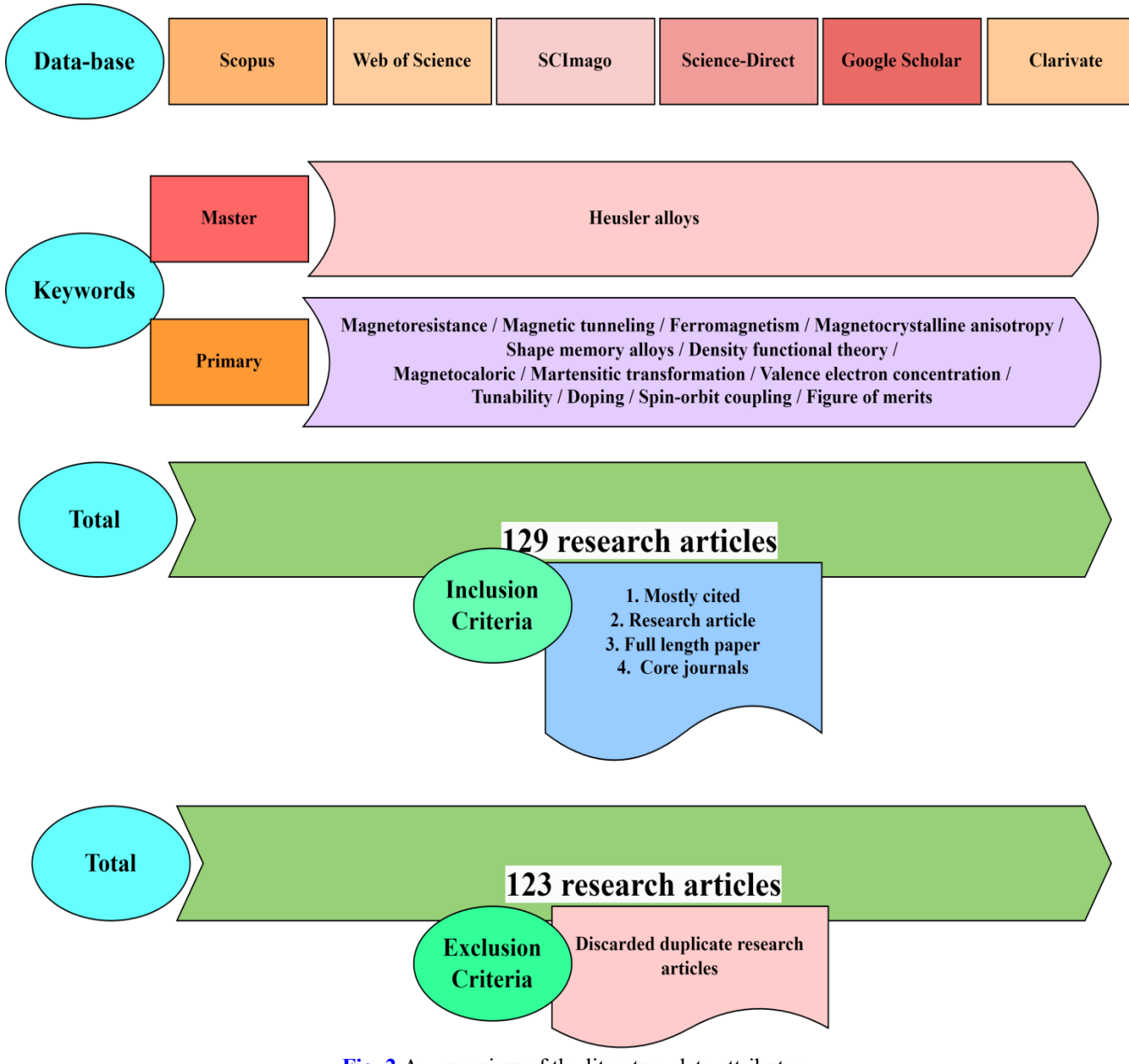

Fig. 2 An overview of the literature data attributes.

4. Network analysis

The open-source software Gephi has facilitated the manipulation and clustering of statistical parameters for the network data. Different journals, authors, years of publication, volume, and publication issues are analyzed using nodes and edges.

The layout utilized is Fruchterman Reingold, with different manual regulations of parametric combinations. Fig. 3 depicts the cluster analysis done on journal titles, authors, and documents with their ISSN, volume, and issue, with the publishing years having 254 nodes and 761 edges. A cluster of the interdisciplinary field of a subject impacting the Heusler alloys research is observed in Fig. 4, having 34 nodes and 52 edges.

4.1 Machine learning algorithm for predictive modeling on the Heusler alloys

Heusler alloys have a broad spectrum of applications; hence, major research works are being done across the globe and are still developing in contemporary research. This research work conceivably laid the foundation for the creative and ingenious development of Heusler alloys to make a breakthrough in condensed matter physics, theoretically and experimentally. Magneto crystalline anisotropy hence signifies a suitable research gap that is henceforth providing critical space to analysts across the scientific community to concentrate research in Heusler alloys, magnetoresistance, magnetocaloric, shape memory alloys, spintronic devices, magneto-mechanical, thermoelectric and magneto crystalline anisotropy. These domains have an imperative scope and therefore need thorough study. The ever-increasing demand for magnetic nanoparticle-based application in magnetic

refrigeration of materials is a potential technique with significant advantages over the currently used gas compression-expansion technique because of its high efficiency and environmental approach; various classes of magnetic nanoparticles are under study. Among them, Heusler alloys, which show half metallicity, is of interest due to substantial spin polarization of 100 % at the Fermi surface. Researchers from India can work on this area of condensed matter physics, which has a great scope to explore and innovate. The family of Heusler compounds are mainly divided into Half Heusler, Full Heusler, and Inverse Heusler compounds. They are referred as intermetallic compounds due to their characteristic atomic order. The authors preferred Half and Full-Heusler compounds because they are basically ternary intermetallic compounds and are easily available in literature as their atomic position, valence electron concentration ratios are proven and observed experimentally and theoretically. Often wrong lattice positions are used in theoretical models leading to wrong results and predictions for other forms of Heusler alloys concerning with the doping of an element without considering the structural compositions.

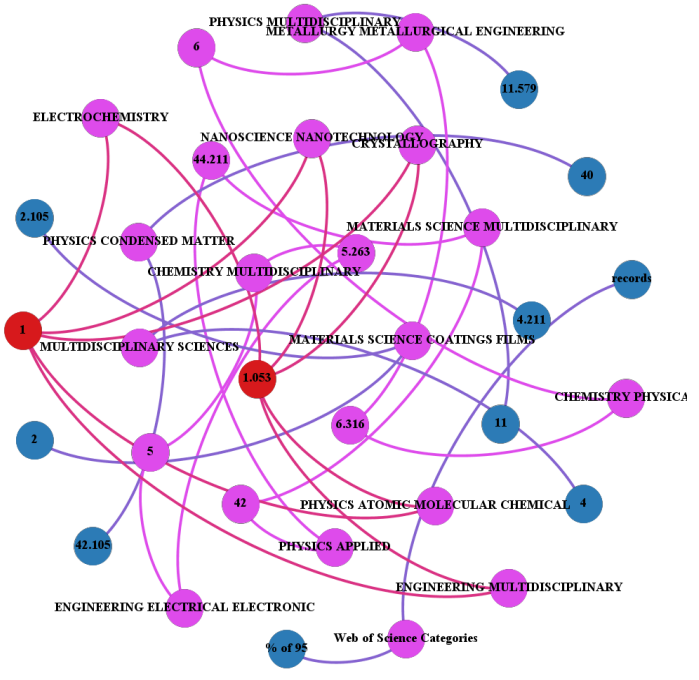

Fig. 3 Cluster of categories co-appearing in the same subject discipline.

Today, extensive portions of the chemical space may be systematically investigated at minimal cost and with high reliability. The computational high-throughput strategy is this.[35,36] Data mining and machine learning techniques have become a part of the material science toolkit as a result of the examination of the generated data. Descriptors, simple proxies for sometimes complex material qualities, and system properties calculated using machine learning regression and classification can all be used to classify materials.[37-39] The latter are especially helpful in cases where a direct computation would be too expensive. In a technique based on machine learning, properties of a particular system are predicted using statistical inference rather than an exact computation of the electronic structure.[40-43]

Machine learning is a logical extension of the computational high-throughput technique since it makes it possible to analyze vast amounts of multidimensional data quickly, objectively, and affordably. Three elements make up machine learning models: (i) a source of training data; (ii) a representation to transform the materials data into a format that is compatible with ML; and (iii) an ML method to develop a function that explains how the representation relates to the material qualities given in the training set. For a specific data set, a single approach might not produce the ideal prediction. Machine learning algorithms have their limitations, and it might be difficult to create a model with high accuracy. We can increase the accuracy overall if we create and connect numerous models. Every primary node in a decision tree or regression tree represents a feature, and each leaf node in a tree-like structure represents a predicted value or class. In a nutshell the primary distinction between a decision tree and a regression tree is the kind of target variable that is predicted. For continuous target variables, a regression tree is employed, and for categorical target variables, a decision tree. The modelling was done to understand the degree of error that can be minimized. The mean square error obtained was different for both the models since the target variable chosen was transition temperature (TT) for regression tree model and valence electron concentration ratio-e/a (EA) for decision tree model. These two variables mainly helps in determining whether the material can be suitable for analyzing its shape memory property.

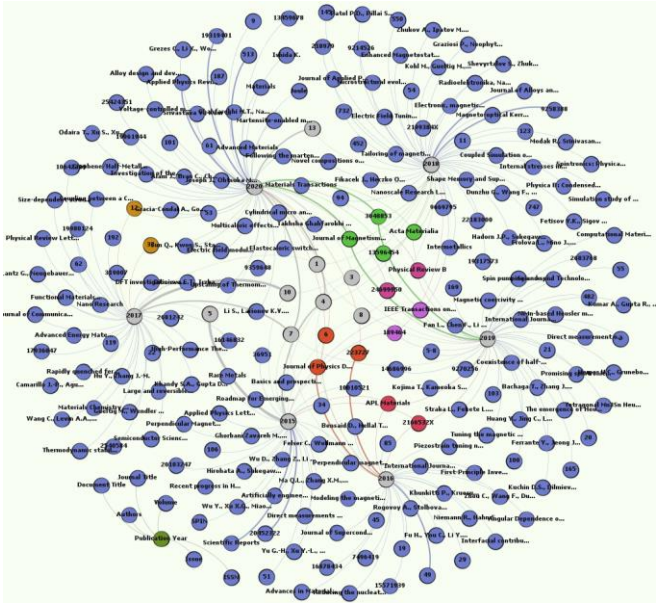

Fig. 4 Cluster of research outputs on core journals.

4.2 Proposing an ML model for designing shape memory alloys

The high temperature cubic phase (austenite) transforms into the tetragonal (martensite) phase in the ferromagnetic state in

the ferromagnetic Heusler alloys with a magnetically controlled shape memory effect. An external magnetic field has the ability to regulate both the structural changes and related processes in these materials. The crystal lattice experiences a spontaneous 20% deformation during the martensitic transition. Superelasticity and a one-way or two-way shape memory effect accompany the martensitic transition. A first-order magneto-structural phase transition can also occur in certain of the Heusler alloys due to the ability of the magnetic and structural transitions to coexist over a significant range of compositions. The alloys in this instance exhibit a massive magnetocaloric effect. For magnetically controlled devices like actuators, sensors, and magnetic freezers operating at room temperature, these aspects make the novel functional materials particularly promising. There is still no comprehensive solution to the underlying physical issue involving the interaction of elastic and magnetic degrees of freedom in the vicinity of phase transitions, despite the fact that since the discovery of this effect in the early 2000s about 10% of strain due to magnetically controlled twin boundary motion in low-temperature tetragonal phase has been attained and may be used commercially. These alloys have the best values of entropy and temperature changes ever observed in magnetic materials for compositions where linked magneto-structural transitions exist. Microscopically, the simultaneous presence of the magnetocaloric and inverse magnetocaloric effects has not yet been fully understood. Therefore, further research is needed to understand the significance of magnetoelastic coupling and magnetic field-driven changes during the martensitic transitions in the ferromagnetic Heusler alloys.

With these factors to be taken into consideration, a machine learning modeling were implemented by choosing the descriptors from the vast multi-dimensional data obtained from the literature sources available in this area through the databases that have been already discussed in this article. Data were extracted from the literature of about 400 results obtained from 75 research articles focusing on ternary Heusler compounds with different stoichiometric compositions with a set of half-Heusler and full-Heusler compounds. A training dataset was created with a group of compounds with various elemental compositions. Most of the entries were Ni-Mn-based Heusler alloys, as they have shown prominent shape memory effect. The total candidates were 300, with 129 (44%) belonging to half-Heusler and the remaining 171 (56%) belonging to full-Heusler. The input features were categorized according to the output characteristics of an SMA. The valence electron concentration (e/a) ratio varies due to the atomic percentages of alloys in the matrix. The SMAs generally exhibit two different phases according to the temperature, such as the martensite phase at lower temperatures and the austenite phase at higher temperatures. The factors that affect the compound formation and mainly control the behavior of alloys include the lattice strain, e/a ratio, stress, difference in entropy, and saturation magnetization. Fig. 5 describes the flowchart for the data extraction process. Fig. 6 gives the block diagram for building a machine-learning model for our problem of interest.

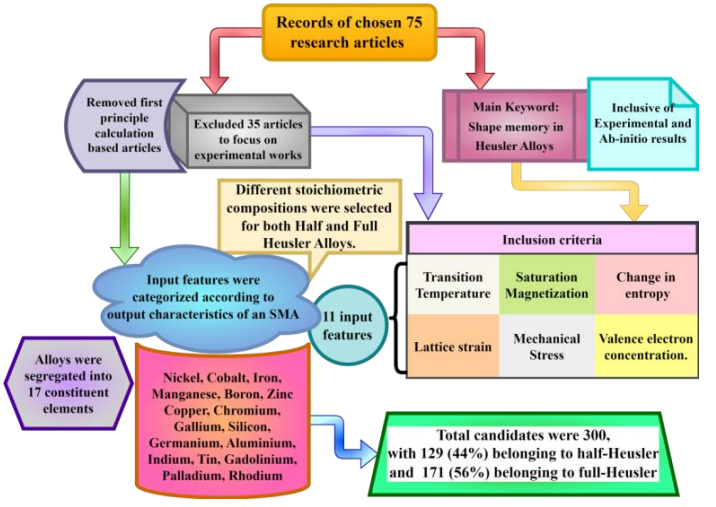

Fig. 5 Flowchart for the data extraction process.

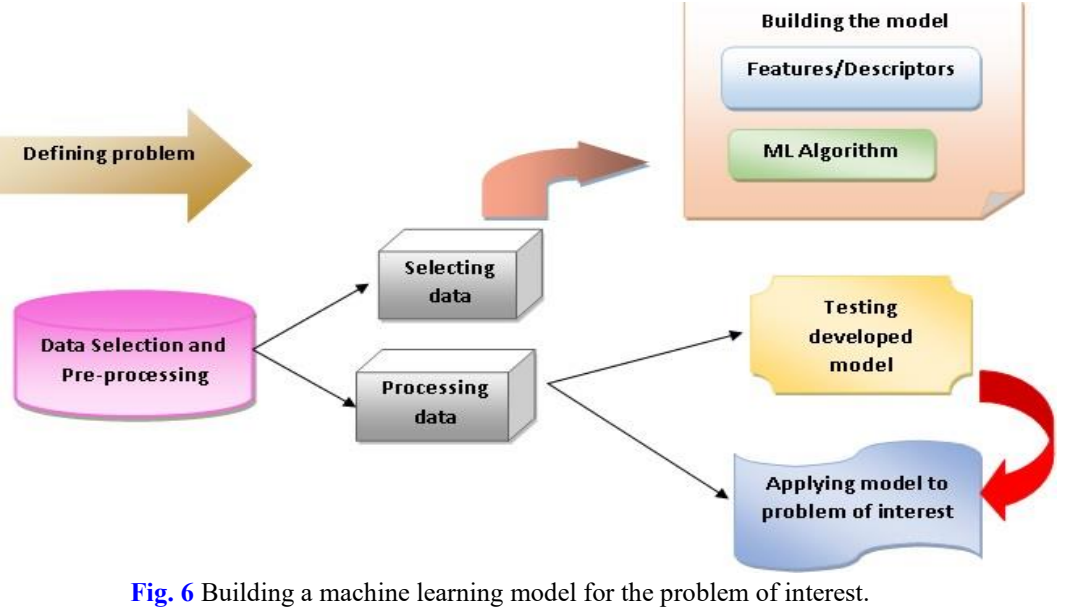

Fig. 6 Building a machine learning model for the problem of interest.

Scikit-learn, a Python module for machine learning, was utilized, and the codes were written and executed in Google Colab. The ML model was built using a decision tree regressor algorithm with a test size of 0.3 and a random state of 100. The prediction engine is run for every input feature, and the testing is done individually. Mean square error (MSE) was estimated for every input feature, and they fell in the range of 0.005 and is shown in Fig. 7. The obtained accuracy of the ML algorithm shows a high degree of correlation between the actual values and predicted values. Decision tree regression is a supervised learning technique. A decision tree is arriving at an estimate by asking a series of questions to the data, each question thus narrowing the possible values until the model gets confident enough to make a single prediction. The model determines the order of the question and the content.

The questions are asked in a True or False form. For each True and False answer, there are separate branches. The root node is the initial node that represents the entire sample and splits it into other nodes. The interior nodes represent the features of a dataset, and the branches represent the decision rules. Leaf nodes represent the outcome. This algorithm is very helpful in solving decision-related problems. Start at the root node on the top and progress through the tree, answering the questions along the way and eventually reaching a prediction. As a supervised machine learning model, a decision tree learns to map data to outputs in the training phase of model building. The model is fitted with the historical data during training, which is relevant to the problem domain and true value. The logic behind splitting the dataset by selecting certain points that best split the dataset is to minimize the mean square error. The points are selected through an iterative process for calculating MSE for all the splits. If there are multiple independent variables at each node, all the variables undergo the same process, and the data is sorted based on each variable separately. MSE is the measure that tells how much the prediction deviates from the original target. It is estimated to be squaring the difference and dividing the entire sum by the total number of records. The basic idea behind the decision tree regression algorithm is to find the point in the independent variable to split the dataset into two parts so that MSE is minimized at that specific point. The algorithm does this in a repetitive mode and forms a tree-like structure.

The same dataset was modeled on the Orange open-source toolkit[44,45] for obtaining a predictive analysis through two workflows developed for regression analysis.

The data sampler widget is useful for sampling the collected data and then producing a complementary dataset. A fixed proportion of data gets sampled for testing and training. A selected number of instances get sampled repetitively to generate more variables. Since the target instance remains one, sampling parametric variables must be continued. It is necessary to have separate datasets for training and testing to avoid overfitting, thus helping correctly predict and model the test scores. Since the model is built based on training data, 70% of the data goes for that, and the remaining 30% is for testing once the model is run.

Further tree widget is implemented, a simple algorithm that can split the data into its branches and nodes by the mean

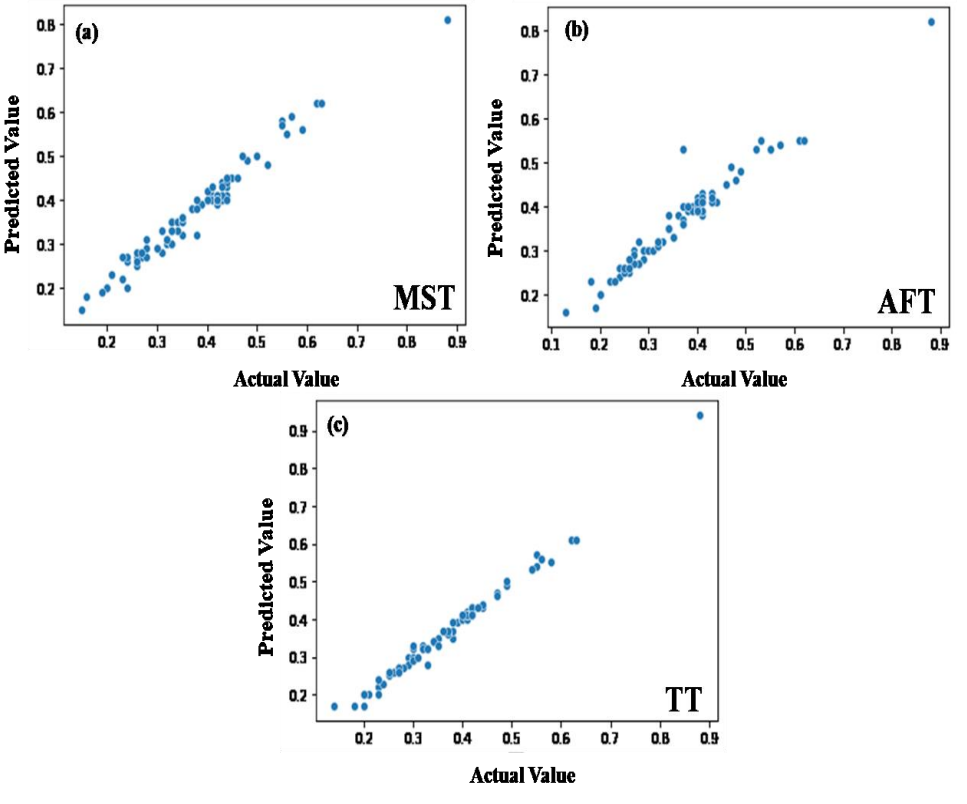

Fig. 7 Comparing the predicted and actual values in terms of (a) Martensitic Start Temperature (MST); (b) Austenitic Finish Temperature (AFT); (c) Transition Temperature (TT).

square error (MSE) for the target numerical variable. It is a pre-processing method and follows a forward-pruning algorithm. Tree viewer is a visualization widget of the same. The test and score widget is where all the computations occur as performance statistics like MSE (*i.e.*, difference between estimator and estimated), RMSE (*i.e.*, measure of imperfection in goodness of fit of the estimator to the data), MAE (a measure that is used to check the closeness of predictions with the outcome) and R^2 (proportion of variance of dependent variable that is predicted from independent variable). k-means widget is a clustering algorithm run on our dataset and gives a new dataset as output where the clusters are labeled to a Meta attribute. Silhouette scores validate the clustering results for various k. If the Silhouette score is between 0.5 to 1, *i.e.*, the higher the silhouette score, the better the clustering and estimates of the quality of clusters formed.

A violin plot depicting data peaks is a cross between a box plot and a kernel density plot. It is used to show how numerical data is distributed. Violin plots provide summary statistics and the density of each variable, unlike box plots, which can only show summary statistics. The white dot indicates the median. The interquartile range is indicated by the broad grey bar in the center. Except for those points that are identified as "outliers" using a technique that is a function of the interquartile range, the thin grey line depicts the remainder of the distribution. The Fig. 8 represents the violin plot. The violin plot is the sum of probability distribution of box plot and kernel density distribution with the differentiation of three clusters. The transition temperature (TT) was augmented is the average of martensitic start temperature (MST) and austenitic finish temperature (AFT). The shape memory is a result of reversible phase transformation and the AST and MST are critical factors that determine the temperature range within which the shape memory effect can be observed. The relationship between the austenitic and martensitic transition temperatures influences the temperature range over which the shape memory effect can be triggered and observed. The relationship between these transition temperatures is central to designing shape memory alloy materials for specific applications. Careful selection of alloy compositions and processing conditions are required to achieve desired transition temperature ranges that align with the intended use of the material. This ensures that the shape memory effect is reliable and functional within the desired temperature range. Hence, the clusters were chosen between these two ranges of temperature. A violin plot consists of "violins," which are symmetrical shapes that represent the distribution of data for each composition. The width of the violin at a given point represents the density of data points at that valence electron concentration. The horizontal line within each violin represents the median valence electron concentration for that composition. By analyzing the violin plot, a pattern or a trend related to the transition temperature and Fe_2NiAl alloy composition.

Figure 8 is the violin plot representing density of every element grouped as three clusters concerning the parameters, transition temperature (TT).

A scatter plot widget is a 2D dimensional visualization for viewing the dataset clusters as scatter plots with certain attributes. Numerical values are represented through blue-

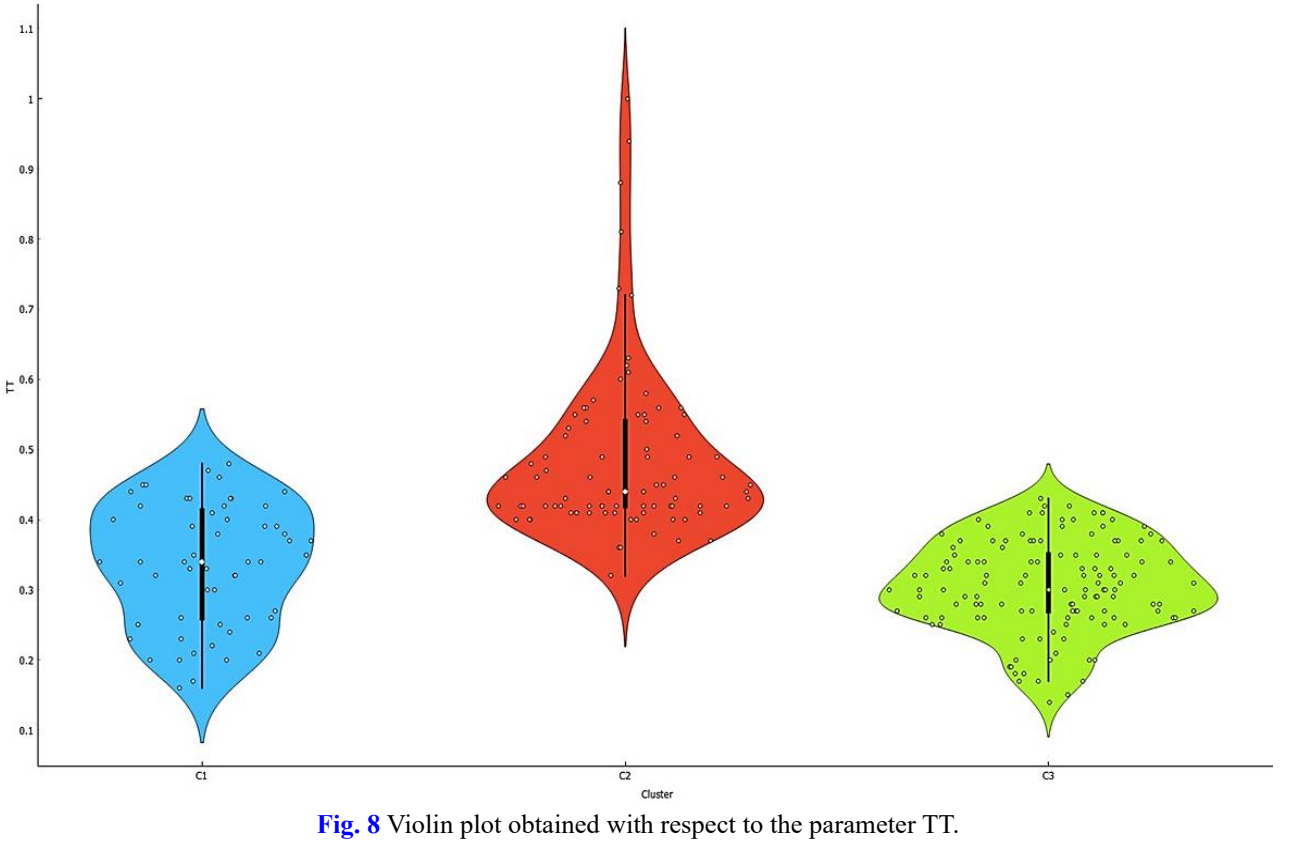

Fig. 8 Violin plot obtained with respect to the parameter TT.

green-yellow color points with labels and shapes to differentiate between points. The opacity of all data points can be chosen through symbols. The jittering can be utilized to prevent overlapping as it randomly scatters the points around the categorical values. The violin plot widget shows the distribution of quantitative data as categorical variables could be compared. For the dataset we created, the violin plot features kernel density estimation for the underlying distribution. The density-Based Spatial Clustering of Applications with Noise (DBSCAN) widget groups the data points that are approximate to each other based on the Euclidean distance, and the algorithm can increase regions into clusters having high density. The clusters are formed with different shapes and sizes from the dataset, even with noise and outliers. When the features other than the target variable are normalized, centered to mean, and scaled to a standard deviation of 1. To display the data's distribution shape, kernel density estimation is placed on either side of the grey line. A larger probability that population members will adopt the provided value is shown by wider areas of the violin plot, whilst a lesser probability is represented by narrower sections. We choose the number of centroids in k-means that represent the number of clusters. Then, each data point will be assigned to its closest centroid (Euclidean) using a distance measure. Unsupervised learning frequently uses the machine learning technique k-means clustering. This technique divides observations into k clusters using the Euclidean distance and assigns each observation to the cluster with the closest mean (cluster centroid). If the dataset has many features, some methods, like k-means, struggle to create clusters with sufficient accuracy (*i.e.*, high dimensionality). It's not always true that high dimensionality entails hundreds or even thousands of features. Accuracy problems can arise with just ten characteristics. The goal of feature or dimensionality reduction is to reduce the number of artificially created features while retaining most of the information in the original features.

Figure 9 is the DBSCAN graph with data points grouped as clusters with the nearest neighbor distance evaluated as 6.44 using the Euclidean distance metric, and the core neighbors chosen were 9.

Using the Local Outlier Factor algorithm is one efficient way to perform outlier detection on moderately high dimensional datasets. The algorithm computes a score reflecting the degree of abnormality of the observations. It measures the local density deviation of a given data point concerning its neighbors. Like many other clustering evaluation metrics, Silhouette Score is subject to error. One must always confirm that the algorithm's distance measure can linearly separate the data before using it to estimate algorithm performance. We must be cautious when quoting silhouette distance in situations when the datasets are not linearly separable, and their dimensions are quite big. Data can be reduced to two dimensions using dimensionality reduction techniques for visualization. As a rule, silhouette distance may not be a suitable metric when utilizing density-based clustering methods. We will be given labeled data in probabilistic and non-probabilistic classification techniques, making it simpler to anticipate the classes. However, we lack knowledge of which data point belongs to which class in the clustering method. The use of distance measures is crucial in this type of method. Table 1 represents silhouette scores obtained for the features that were characterized as input descriptors that determined the performance of model. 9th instance has been chosen as the root node from the 30 instances developed from 70% of the testing run on data from the total 300 datasets. The predictive score obtained was 0.61, and it is because of the relatively higher value of its major target variable NIC. Then moved down to the tree branch and got split at the 5th instance with a predictive score of 0.51. The process continues until it reaches a specified majority threshold. The tree has formed through the major target variable NIC as the data collected after pruning had more instances with Nickel (NIC) as the main element and the primary feature variable among the 27 variables in the chosen Heusler alloys. Table 2 gives the prediction metrics that were utilized to check the accuracy of our predictions and convey the numeral deviation from actual values. The mean square error (MSE), root mean square error (RMSE), mean absolute error (MAE), and R^2 are all measures used to assess the model's effectiveness in regression analysis. MSE is the average squared difference between the original and predicted values in the dataset. In contrast, MAE is the average of the absolute error difference between the actual and anticipated values in the dataset, *i.e.*, assessing the variance of the residuals. RMSE measures the standard deviation of the residuals. R^2 measures how well a regression model fits a dataset and how well it reproduces observed findings based on the proportion of total variation in outcomes that the model is responsible for explaining.

Table 1. Features with their Silhouette scores.

Features	Silhouette scores
MST	0.344
MFT	0.318
AST	0.351
AFT	0.345
TT	0.348
LS	0.396
STR	0.396
SM	0.388
EC	0.390

Table 2. Metrics obtained from Regression Model.

Model	MSE	RMSE	MAE	R2
Tree	0.004	0.067	0.043	0.740

The machine learning model is also utilized to discover Heusler compounds magnetic intermetallic proposed for applications other than shape memory alloys. Knowledge of crystal structures is necessary to enhance the electrical and

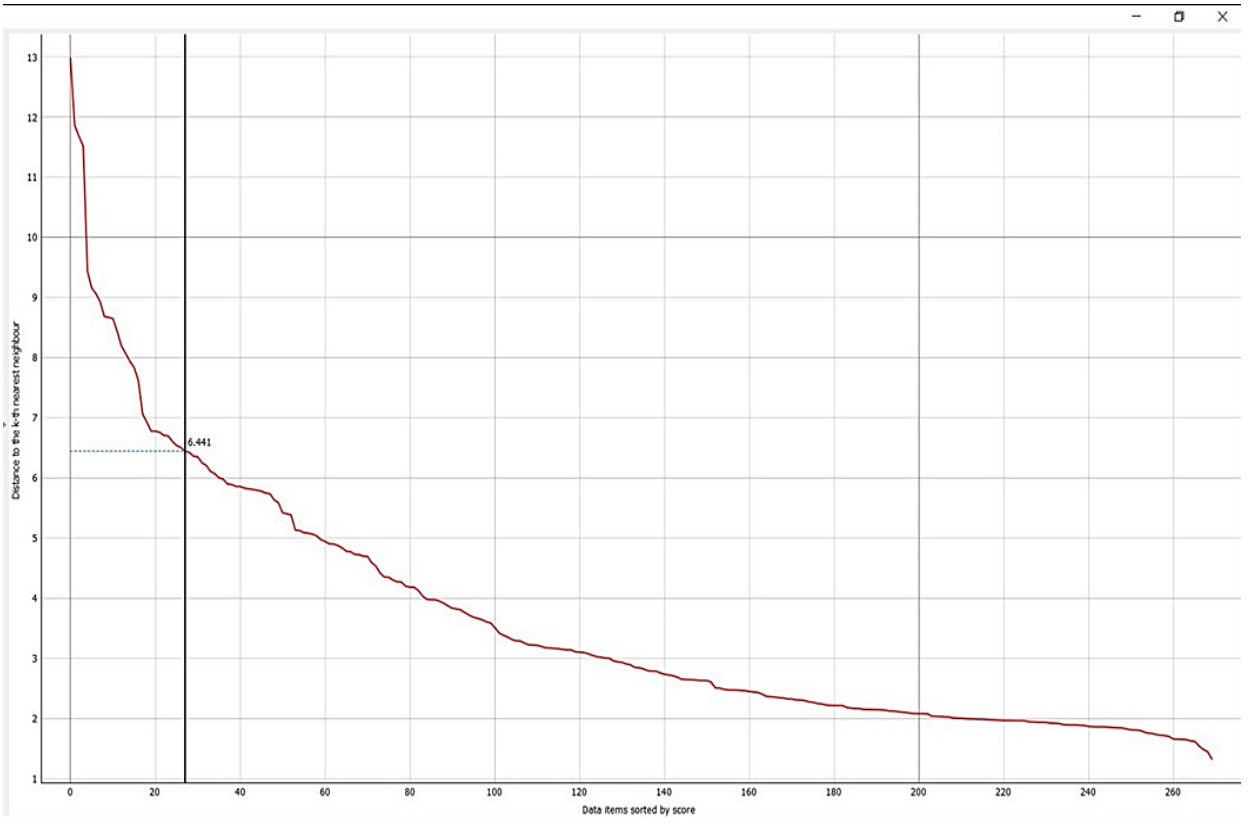

Fig. 9 DBSCAN graph based on Euclidean distance metric for the nine input variables of Has.

magnetic properties. They exist in three forms like Heusler, inverse Heusler, and CsCl-type structures, and to distinguish each other, diffraction techniques are insufficient, and these structures seem endlessly complicated. Perhaps with synchrotron radiation, XRD can make a distinction between the structures. Single-crystal XRD is a better accurate method, but only 2% of compounds distinguish Heusler and inverse Heusler structures. Determining the correct structures of these compounds is vitally crucial to improving their performance in materials applications because subtle structural differences can significantly influence their multifunctional properties. These all-interesting facts make an impact as the expectations and outlook on HAs seem to be intense and insightful. There has been promising progress made in preparing Heusler nanoparticles, yet there is a need to have a facile and robust synthesis approach to developing high-quality Heusler nanoparticles. So far, the theoretical and experimental studies on the surface effects of physical properties of Heusler alloy nanoparticles. The half-metallic characteristic of magnetic nanoparticles can be conserved by changing the surface modifications as it can be compared with bulk. So far, no spin-related transport measurements have been conducted. Recently, an extraordinary development has been made in the nanofabrication technique, illustrating the direct measurement of the intrinsic spin polarization of Fe-Co-Si nanowires that can be utilized for magnetic storage devices. First principal calculations are proven effective in studying the size-dependent electronic and magnetic properties in magnetic semiconducting nanocrystals. Ni-Mn-Ga Heusler shape memory alloys face difficulties in industrial applications due to the brittleness, low working temperature and intricacy of production and hence the need for a new ferromagnetic shape memory Heusler alloys have been investigated to prevail these challenges along with exploring thermoelastic properties as well as stimulating a change in bulk modulus to have a martensitic transformation applied on to the conventional shape memory alloys (SMAs). The grain size is smaller than the critical size associated with a thermally induced superparamagnetic limit. Novel multifunctional properties such as super elasticity, ductility, and high energy damping can be found in single ferrous polycrystalline ferromagnetic SMAs. Substantially, new Heusler shape memory nanoparticles are an implication of next-generation miniaturized medical devices, actuators, and sensors by exhibiting robust shape memory properties that can break the constraints put forward based on grain size, which seems to be comparable to that of superparamagnetic limit. Basically, for any of the spintronic applications, thin films of Heusler alloys are preferred. Thus, plenty of research is being focused on the theoretical aspects to study the electronic structure and the density of states that prevail in the half-metallic behavior of HA thin films and the technological aspect that aimed at the fabrication of thin films with the highest spin polarization at optimum conditions. The development and formation of HA thin films are challenging as the difficulty lies in properly ordering different elements into the four sub-lattices. Antisite disorder is one of the defects that can affect the spin polarization as well as the Curie temperature of the ferromagnetic ternary alloys resulting in the

failure of achieving 100% polarization in nanostructures containing HA layers and another difficulty occurs in the preparation of HA films that can manifest ferromagnetic shape memory effect.

5. Conclusion and future scope

This article was made on contemporary developments in Heusler alloys and has shown that immense publications have come from articles, review papers, and conference papers related to physics and chemistry due to their accessibility and the profound connection of multifunctional properties to the topic of research and also being affiliated to material sciences. Researchers worldwide are showing zealous curiosity on this topic, making it a large and substantial arena to be focused upon. Heusler alloys are a niche area of interest in condensed matter physics experimentally and theoretically. To make good quality Heusler alloy nanoparticles, appropriate top-down or bottom-up synthesis techniques must be implemented. There are only a few reports of successful, high-quality preparation of Heusler nanoparticles via the bottom-up approach. Heusler alloys are a distinct class of materials whose compositions can be changed without structural change. First, density functional calculations are being implemented to determine the structural, mechanical, electronic, optical, and thermoelectric properties of Heusler alloys through various software packages like DFTB+, GAMESS, ORCA, Quantum Espresso, Siesta, and VASP. Numerous characterization techniques are utilized in the research process and reveal the structural, physical, chemical, and magnetic properties of synthesized Heusler nanoparticles. Machine learning uses statistical inferences to predict properties without performing electronic structure estimations. Machine learning has the potential to discover new materials and substitute stoichiometric compounds. Even machine learning algorithms train experimental data to unravel the probability that a given XYZ stoichiometry adopts either Half or Full Heusler structures. In recent times, material scientists worldwide have embraced machine learning to achieve data-driven optimization in their respective research fields. This has created a strong platform for computational materials science, providing unambiguous support through open-source tools and data-sharing. This truly revolutionizes the vast area of materials science by making a path for discovering new materials that can reduce arduous experimentations and inevitable characterization studies. The use of machine learning is of particular importance in Heusler alloys as these alloys can have a variety of components, thus resulting in various properties and applications. Future years will undoubtedly see the emergence of numerous exciting research initiatives that make use of their infinite functions. When several Heusler materials are deposited on top of one another, a device is created that responds differently to different external forces. For example, applying a current to a half-metallic ferromagnet causes a spin injection into the semiconducting Heusler compound, or applying a magnetic field to a shape memory alloy can cause it to deform and affect how the topological insulator behaves. Within one material class, the Heusler compounds, such a device could be created in accordance with the unique requirements of the relevant application and the novel, unidentified multifunctional characteristics could be created.

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Conflict of Interest

There is no conflict of interest.

Supporting Information

Not applicable.

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