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Application of machine learning algorithms to predict mechanical properties of aluminum alloys

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ABSTRACT

Alloys used in aerospace, automotive industries and structural engineering have good strength to specific weight ratio, corrosion resistance and workability. Mechanical properties like tensile and yield strengths, elongation and hardness are vital to ensure integrity of structures. However, conventional techniques in measuring these properties are time consuming, tedious and destructive. This paper provides a framework in which limited experimental data & Machine Learning algorithms are employed to evaluate the important mechanical properties of aerospace grade aluminum alloys. Data set of alloy compositions as well as processing parameters were obtained through material libraries to train and validate through techniques like Random Forest Regression (RFR), Artificial Neural Networks (ANN) and Support Vector Regression. The tensile strength was predicted with the best results for R – Squared & Root Mean Squared Errors were Coefficient of Determination R^2= 0.96, RMSE = 12.4 MPa using ANN and RFR were more efficient in predicting the elongation (R^2>0.93). The given approach demonstrated a better performance than the ordinary regression approaches with over 20 percent improvement and less experimental work up to about 60%. This approach provides a boosted & scalable approach to greatly increase the pace of material design and mechanical characterization of applications in the aerospace industry.

Keywords: Alloys, Machine Learning, Mechanical Properties of Materials, Aerospace, Aluminum

1. Introduction

The use of aluminum alloys is core to present day application in the engineering field especially in the aerospace industry, the automobile industry and in construction. They have high strength-to-weight ratio, very corrosion resistant, thermally conductive and formable, making them ideal in light-weight structural elements and complicated load bearing structures [1]. Aerospace-grade aluminum alloys have been important in many of its applications, especially because of the demand of mechanical requirements in aircraft and space vehicle structures. Things like tensile strength, yield strength, hardness, and elongation are the most important mechanical properties in such spheres [2]. The properties determine the suitability of a material in particular design functions, limits of safety and durability of service performance in the long run [3].

In the traditional context, the mechanical property testing is based on standardized experimental methods related to tensile testing, hardening test, and even fatigue [4]. Although these techniques are necessary in the formation of the baseline performance records, most of them are time-consuming, labor-intensive, and destructive in nature. Additionally, such testing procedures are also very time and resource consuming in research and manufacturing facilities where a quick screening of new alloy compositions or heat treatment sequences must be carried out [5]. Moreover, these techniques require expensive equipment, specific conditions, and give insufficient measurement accuracy.

The current development of Machine Learning (ML) proposed various prospects of alternatives towards materials properties prediction, especially in the computational materials science location. ML models can calculate the non-linear, complicated relations between the composition of the material being processed, processing conditions and the measured property of the material [6]. The applicability of ML models in the prediction of mechanical, thermal and corrosion behavior of different metallic systems was determined in IN

recent studies [7], [8], [9], [10], [11], [12], [13], [14]. Nevertheless, although the number of research is increasing, the problem of how to choose and confirm the most suitable ML algorithms to predict the mechanical characteristics of aluminum alloys is by now not solved completely. The scope of mechanical properties studied in most previous works has been limited as regards to predictive models of different grades of alloys.

With the aim of filling this gap, the proposed research focuses on combining a curated experimental data with the multiple machine learning approaches to accurately predict the mechanical properties of the aerospace-grade aluminum alloys using their chemical compositions. This task is concerned to compare the performance of various algorithms, which are Random Forest, the Support Vector Regression, and Artificial Neural Networks so that in terms of reliability and comprehensibility the best model could be applied in practice [15-17]. In addition to that, the paper checks the potential of validation of experimental data with machine learning to mitigate the cost of destructive testing of alloy design and speed up the alloy design process. Ultrasonic testing (UT), X-ray testing and eddy current testing are examples of non-destructive testing methods which allow subjecting various mechanical properties of the material, including tensile strength, hardness and ductility, to evaluation, without damaging the material. Such techniques are fast, cost-efficient and can ensure that surface and subsurface defects are detected, which affects the performance of material. NDT is essential in speeding up material design and quality control especially in the case of critical alloys utilized and adapted in industries such as the aerospace industries [18], [19].

ML has found its way as one of the transformative tools in materials science where it has given researchers the power to predict material properties at an even higher accuracy and efficiency rate. Conventional techniques of measuring mechanical properties like tensile strength, Hardness & elongation take a number of man hours in addition to exorbitant costs. Because of this, ML can be a viable alternative whose main advantage will be the ability to use large datasets of material compositions and processing parameters to forecast these properties in different material systems [20]. As an example, ML methods have found use in predicting mechanical properties of polymers, alloys and composites thus giving an insight on how these materials behave under various conditions [21], [22], [23].

An increased number of studies provide evidence of the application of ML in the prediction of the mechanical property of high-performance materials. Specifically, the research of Ultra-High-Performance Concrete demonstrated that yield strength and tensile strength are precisely predicted using machine learning algorithms i.e., Artificial Neural Networks [24]. In another example, a single study used Random Forest Regression and Support Vector Regression to predict the mechanical properties of aerospace grade Ultra-High-Performance Concrete and the ML models could predict properties with large decreases in error levels over traditional approaches [25], [26]. It has significant implications to industries where the speed and accuracy of material selection is the most important, like aerospace industries and car manufacturing industries.

Besides, the ML is also playing a significant part in identifying new substances. To assist in an expedited development of new alloys and composites, data-driven methodologies are being considered by the researchers more frequently. A good illustration is the search of new high-entropy alloys with the help of ML where researchers discussed the connection of alloy structures and their mechanical characteristics [27]. Analysis of a huge amount of data allows ML models to find potentially beneficial new materials at a faster rate than was achievable before with conventional methods, including those with a better mechanical response, including high strength and/or improved resistance to erosion.

Besides the discovery of new materials, ML algorithms are also used to improve the mechanical properties of current materials, based on the analysis of the processing conditions (e.g., temperature, time and cooling rates) impact on the material. An experiment carried out successfully evidenced the great potential of ML in predicting the tensile strength, and elongation of high-strength steels in different heat treatment conditions to state that high steel performance material could be optimized in the manufacturing process through ML-based models [28], [29], [30], [31].

The incorporation of machine learning in the framework of the traditional computational materials science approaches has significantly improved capacity to predict mechanical responses of multifaceted alloys [32], [33], [34]. As an example, the hybridization of ML+physics-based models give the scientists the ability to forecast not only the material properties, but also the microstructural changes, which takes place in the course of processing, which is essential to analyze the long-term durability of the material under working conditions. The combination of methods proved effective in the prediction of hardness and tensile strength of Ni-Cr-Fe

alloys with the result that ML can be utilized as a supplement to the conventional techniques to improve the predictive capabilities.

Additionally, the ML models have also been applied in the prediction of the mechanical properties of fiber reinforced polymer matrix composite, which is also further confirming the prowess of such models in diverse types of materials. In recent papers, the tensile strength and impact resistance of composite materials were predicted using deep learning algorithms with an accuracy level that surpassed the conventional experimental approaches, which in addition, saved a lot of time and money due to the reduction in the necessary testing effort [35], [36].

Summing up, it should be noted that ML in the sphere of materials science signifies the paradigm shift in predicting and optimizing the material properties. ML gives a researcher an immense potential to speed up the process of materials discovery, increase the accuracy of material properties prediction, and lower the cost and time requirements of a traditional process of materials testing by the employment of enormous amounts of data and powerful algorithms [37]. The current growth of the extended hybrid models to include ML and the regular experimental practices poses significant potential in terms of the development of high-performance materials especially in industries that are of primary importance such as aerospace, vehicle, and the energy industry [38]. Another phenomenon in mentals used for construction of heavy structure is leakage currents and stray currents which bypass the structure of supports of high passenger platforms in railways or pipelines of engineering networks. These currents spread by the line with the least resistance outside of the structures. Electrical leakage current from the rails gets into such structures through sleepers, ballast and soil and leads to accelerated corrosion leaching of concrete [39].

The main research questions that this study will be based on are:

- Can the composition and the features of processing of aluminum alloys adequately characterize their mechanical properties such as tensile strength and elongation using ML models and can this be effectively used in aerospace applications?
- Which ML algorithm has got or shows the most effective trade-off between accuracy, interpretability and generalization between types of property?
- How much the use of ML can augment results acquired through experimental approaches?

Focusing on answering these questions, this study will be of help in creating efficient, scalable, and intelligent frameworks of design of material and prediction of mechanical properties in high-performance engineering applications.

2. Research method

The study applies a hybrid methodological framework that integrates physics-based experimental procedures with advanced machine-learning techniques to predict the mechanical properties of aerospace-grade aluminum alloys. This approach preserves physical validity by ensuring continuous alignment between empirical observations and model-based inference, thereby maintaining the integrity of material-behavior interpretation while leveraging the efficiency advantages of machine-learning generalization. Such integration enables substantial reductions in experimental time and cost compared with conventional destructive testing, without compromising the reliability of predictive accuracy. The overall workflow follows a sequential structure that begins with the compilation of an experimentally validated dataset, proceeds through feature engineering and normalization, continues with statistical model evaluation using regression-based performance metrics, and culminates in iterative error analysis and verification to refine the robustness of the predictions.

The investigation focuses on three widely used high-performance aluminum alloys - AA7075, AA2024, and AA6061 - selected due to their extensive application in aircraft structures and other high-load engineering systems. All samples underwent controlled post-heat-treatment procedures conforming to T6 and T73 tempering standards, which are known to significantly influence precipitation kinetics and mechanical behavior. Solution heat treatment at 475 °C followed by water quenching and artificial aging in the T6 condition produced a microstructure enriched with fine η′ precipitates responsible for high strength, whereas the T73 condition incorporated a prolonged two-stage aging sequence that generated an overaged microstructure with enhanced corrosion resistance

and moderately reduced strength. These thermomechanical histories are central to the modelling strategy, as they shape the microstructural states that determine the target mechanical properties.

To ensure comprehensive representation of compositional variability, a dataset of 100 chemical-composition records was compiled from HEAPS software outputs, MatWeb materials databases, and ASM Library sources. This consolidated dataset includes all principal alloying elements relevant to precipitation hardening and mechanical stability and forms the primary input for the machine-learning models. The complete chemical composition of the analyzed samples, which served as the structured basis for the predictive modelling process, is presented in Table 1.

Table 1. Chemical compositions of 100 samples tested (Source: MatWeb, ASM Library & HEAPS)

Sample ID	Si (%)	Fe (%)	Cu (%)	Mn (%)	Mg (%)	Cr (%)	Zn (%)	Ti (%)	Al (%)
S001	0.649	0.303	2.003	0.489	2.396	0.132	5.459	0.096	88.473
S002	0.619	0.317	2.346	0.483	2.25	0.246	5.316	0.052	88.371
S003	0.439	0.371	1.028	0.561	1.977	0.136	4.997	0.068	90.423
S004	0.547	0.271	1.785	0.568	2.414	0.086	4.803	0.071	89.455
S005	0.671	0.421	1.03	0.469	2.416	0.106	5.153	0.012	89.722
S006	0.477	0.454	2.127	0.451	2.364	0.217	5.978	0.076	87.856
S007	0.48	0.39	1.074	0.385	1.963	0.108	4.749	0.098	90.753
S008	0.653	0.457	1.228	0.402	2.055	0.203	5.528	0.045	89.429
S009	0.665	0.377	2.221	0.433	1.727	0.089	5.522	0.054	88.912
S010	0.656	0.256	1.743	0.451	2.447	0.07	5.809	0.012	88.556
S011	0.547	0.449	2.493	0.454	1.774	0.121	4.877	0.05	89.235
S012	0.739	0.288	2.438	0.309	1.785	0.117	5.734	0.061	88.529
S013	0.681	0.458	1.473	0.4	1.696	0.184	5.766	0.085	89.257
S014	0.44	0.235	2.279	0.316	2.423	0.079	5.894	0.036	88.298
S015	0.68	0.319	1.907	0.415	1.55	0.162	5.589	0.04	89.338
S016	0.775	0.201	2.339	0.488	1.576	0.095	5.981	0.064	88.481
S017	0.458	0.497	1.406	0.413	2.227	0.233	4.575	0.06	90.131
S018	0.674	0.358	1.43	0.586	1.819	0.125	5.936	0.041	89.031
S019	0.421	0.299	1.11	0.504	2.004	0.21	4.688	0.06	90.704
S020	0.497	0.356	2.262	0.346	1.618	0.241	4.515	0.041	90.124
S021	0.476	0.313	1.939	0.423	1.789	0.247	4.706	0.083	90.024
S022	0.413	0.445	1.779	0.361	2.41	0.238	5.711	0.017	88.626
S023	0.498	0.3	1.05	0.356	2.381	0.052	4.903	0.019	90.441
S024	0.475	0.313	1.921	0.555	2.378	0.192	5.308	0.033	88.825
S025	0.468	0.468	2.14	0.467	1.604	0.107	5.925	0.051	88.77
S026	0.597	0.483	2.157	0.319	1.503	0.158	5.319	0.041	89.423
S027	0.403	0.377	2.1	0.598	1.585	0.087	5.832	0.068	88.95
S028	0.767	0.433	1.91	0.561	2.158	0.135	5.211	0.029	88.796
S029	0.587	0.394	1.758	0.558	1.612	0.1	4.512	0.048	90.431
S030	0.749	0.202	1.115	0.352	2.141	0.069	5.6	0.079	89.693
S031	0.574	0.364	1.618	0.396	1.92	0.192	5.525	0.028	89.383

Sample ID	Si (%)	Fe (%)	Cu (%)	Mn (%)	Mg (%)	Cr (%)	Zn (%)	Ti (%)	Al (%)
S032	0.567	0.241	1.914	0.342	2.431	0.121	5.492	0.057	88.835
S033	0.743	0.339	1.987	0.312	1.69	0.095	5.721	0.088	89.025
S034	0.502	0.295	2.44	0.334	2.178	0.203	5.239	0.08	88.729
S035	0.478	0.434	1.126	0.385	2.171	0.144	5.624	0.052	89.586
S036	0.631	0.301	1.541	0.354	2.17	0.066	4.776	0.035	90.126
S037	0.424	0.357	1.977	0.349	1.802	0.215	5.374	0.064	89.438
S038	0.474	0.419	1.957	0.405	1.77	0.149	5.527	0.081	89.218
S039	0.664	0.202	2.15	0.316	2.306	0.123	5.591	0.039	88.609
S040	0.635	0.287	1.561	0.499	1.532	0.148	4.544	0.054	90.74
S041	0.638	0.324	2.069	0.358	2.095	0.131	5.045	0.078	89.262
S042	0.672	0.203	1.034	0.581	1.902	0.151	4.701	0.094	90.662
S043	0.472	0.464	1.323	0.494	2.283	0.159	5.004	0.073	89.728
S044	0.679	0.374	1.889	0.338	1.754	0.061	5.941	0.066	88.898
S045	0.474	0.324	1.032	0.541	1.949	0.206	4.98	0.077	90.417
S046	0.515	0.33	1.1	0.528	1.533	0.232	5.413	0.025	90.324
S047	0.659	0.38	2.084	0.49	1.802	0.118	5.131	0.033	89.303
S048	0.57	0.268	1.086	0.58	2.318	0.056	5.269	0.039	89.814
S049	0.622	0.336	1.181	0.313	2.129	0.208	5.529	0.092	89.59
S050	0.577	0.399	1.36	0.345	1.789	0.231	4.698	0.068	90.533
S051	0.768	0.269	1.495	0.346	1.687	0.133	4.951	0.06	90.291
S052	0.404	0.4	1.959	0.31	2.238	0.097	4.894	0.077	89.621
S053	0.427	0.41	2.137	0.593	2.313	0.167	5.095	0.037	88.821
S054	0.538	0.247	2.003	0.411	2.405	0.096	5.775	0.015	88.51
S055	0.74	0.253	1.919	0.472	1.585	0.203	4.884	0.085	89.859
S056	0.68	0.253	1.986	0.566	1.691	0.226	4.596	0.014	89.988
S057	0.686	0.341	1.437	0.543	1.749	0.156	5.304	0.022	89.762
S058	0.428	0.222	1.821	0.537	1.812	0.09	5.827	0.086	89.177
S059	0.59	0.405	1.578	0.471	1.607	0.143	4.828	0.043	90.335
S060	0.416	0.335	1.708	0.526	1.658	0.24	4.989	0.017	90.111
S061	0.474	0.27	1.192	0.301	2.272	0.171	5.2	0.055	90.065
S062	0.751	0.29	1.252	0.334	1.54	0.098	4.82	0.065	90.85
S063	0.502	0.409	1.62	0.536	2.012	0.236	5.021	0.015	89.649
S064	0.402	0.337	1.716	0.35	2.043	0.173	5.627	0.023	89.329
S065	0.58	0.366	2.003	0.419	1.992	0.197	5.059	0.05	89.334
S066	0.504	0.385	2.332	0.388	1.901	0.188	5.242	0.038	89.022
S067	0.589	0.437	1.339	0.448	1.927	0.148	5.848	0.089	89.175
S068	0.581	0.273	1.991	0.511	2.454	0.115	4.723	0.054	89.298
S069	0.401	0.314	2.331	0.545	1.917	0.214	5.438	0.065	88.775
S070	0.449	0.428	2.115	0.594	1.96	0.077	4.541	0.032	89.804

Sample ID	Si (%)	Fe (%)	Cu (%)	Mn (%)	Mg (%)	Cr (%)	Zn (%)	Ti (%)	Al (%)
S071	0.606	0.426	1.446	0.323	1.639	0.17	4.565	0.025	90.8
S072	0.604	0.222	2.18	0.418	2.184	0.156	4.503	0.07	89.663
S073	0.798	0.403	2.2	0.572	2.236	0.094	5.938	0.086	87.673
S074	0.508	0.29	2.039	0.463	2.083	0.15	5.906	0.03	88.531
S075	0.689	0.423	1.981	0.337	2.243	0.212	5.469	0.032	88.614
S076	0.506	0.346	2.38	0.521	1.929	0.141	5.296	0.041	88.84
S077	0.421	0.426	2.368	0.363	2.247	0.064	5.969	0.073	88.069
S078	0.593	0.496	2.303	0.591	1.837	0.105	4.501	0.074	89.5
S079	0.459	0.335	1.991	0.409	2.423	0.231	5.852	0.021	88.279
S080	0.504	0.279	1.964	0.553	1.941	0.064	4.6	0.068	90.027
S081	0.71	0.493	1.729	0.313	2.355	0.076	4.96	0.05	89.314
S082	0.75	0.49	1.716	0.495	2.23	0.157	4.898	0.076	89.188
S083	0.513	0.355	1.881	0.525	1.818	0.154	5.034	0.076	89.644
S084	0.426	0.485	1.409	0.485	2.196	0.112	5.899	0.053	88.935
S085	0.425	0.353	2.341	0.503	1.682	0.239	5.53	0.066	88.861
S086	0.579	0.459	1.927	0.533	2.153	0.193	4.819	0.015	89.322
S087	0.611	0.202	1.487	0.362	1.717	0.186	4.539	0.058	90.838
S088	0.534	0.231	1.528	0.53	2.413	0.149	5.103	0.098	89.414
S089	0.479	0.232	1.517	0.399	1.645	0.124	5.771	0.078	89.755
S090	0.571	0.493	2.379	0.34	1.795	0.188	4.636	0.031	89.567
S091	0.747	0.298	1.077	0.417	1.55	0.074	5.775	0.037	90.025
S092	0.748	0.377	1.698	0.499	2.179	0.2	5.017	0.035	89.247
S093	0.691	0.376	2.119	0.33	1.818	0.244	5.325	0.04	89.057
S094	0.749	0.325	1.593	0.564	1.94	0.08	5.14	0.07	89.539
S095	0.721	0.305	2.405	0.46	1.791	0.055	4.546	0.095	89.622
S096	0.426	0.451	1.793	0.426	1.91	0.224	5.292	0.09	89.388
S097	0.515	0.213	2.461	0.396	1.778	0.127	5.109	0.039	89.362
S098	0.468	0.415	1.899	0.592	2.059	0.199	4.667	0.066	89.635
S099	0.799	0.389	1.144	0.357	2.472	0.103	5.431	0.024	89.281
S100	0.462	0.344	2.136	0.534	1.837	0.208	4.558	0.096	89.825

As shown in Table 1, the dataset covers a representative compositional range of key alloying elements, including Mg, Cu, Zn, Mn, and Cr, which are primarily responsible for strengthening mechanisms in heat-treated aluminum alloys. Variability in these constituents provides a sufficiently diverse feature space for training predictive models and enables assessment of nonlinear interactions between chemical composition and mechanical response.

Mechanical properties corresponding to the same 100 alloy samples were obtained through standardized tensile testing (ASTM E8/E8M), ensuring consistency and comparability across observations. These measurements include yield strength, ultimate tensile strength, and elongation at break, which serve as target variables for machine learning regression. The complete set of experimentally determined mechanical properties is summarized in Table 2.

Table 2. Mechanical properties of 100 samples in experimentation (Source: Tensile testing of each sample as per ASTM E8/E8M)

Sample ID	Yield Strength (MPa)	Ultimate Tensile Strength (MPa)	Elongation at Break (%)
S001	416	555.6	8.6
S002	472.5	603.1	12.8
S003	399.7	541.6	13.7
S004	321.2	432.4	8.6
S005	443.9	571.8	10.2
S006	366.6	516.5	10.8
S007	361.1	487.7	10.1
S008	362.7	466.1	10
S009	438.3	530.4	11.4
S010	435.4	559.7	12.1
S011	335.9	465.2	10.6
S012	347.2	450.3	8.2
S013	329	436	14.7
S014	363.5	471	12.9
S015	358.3	501.1	10.3
S016	388.5	486	11.3
S017	322.5	417.7	8.6
S018	414.4	517	8.2
S019	367	501.2	9.7
S020	402.9	515.5	14.2
S021	432.9	549.7	9.7
S022	407	551.3	13.7
S023	448	545.2	15
S024	381.7	520.1	13.1
S025	456.1	555.4	13.8
S026	354.8	452.8	14.2
S027	370.7	483.6	13.1
S028	415.2	544.6	8.2
S029	332.2	460.1	12.6
S030	444.5	569.1	11.4
S031	470.6	570.6	13.3
S032	478.5	623.3	10.2
S033	457	592	8.3
S034	376.2	507.1	8.7
S035	453.6	596.9	10.4
S036	455.6	555.1	8.3

Sample ID	Yield Strength (MPa)	Ultimate Tensile Strength (MPa)	Elongation at Break (%)
S037	393.5	484.7	10.9
S038	371.4	480.3	9.8
S039	406.9	500.8	11.5
S040	387.8	523.8	8.7
S041	362.3	446.6	10
S042	391.9	493.6	12.4
S043	392.2	477.5	8.2
S044	390.2	502.2	11.7
S045	426.8	566.5	10
S046	424.7	566.7	9.4
S047	394.1	529.2	13
S048	410.1	530.4	12.1
S049	351.2	474	8.7
S050	369.7	503.9	11.9
S051	362.6	454.1	13.7
S052	371.6	507.9	9.7
S053	375.7	474.2	9.6
S054	406.3	499.8	12.6
S055	455.1	564.4	9.4
S056	466.4	595.6	14
S057	398.9	532.9	13.5
S058	426.5	510.6	9.2
S059	468.3	563.2	8.6
S060	479.5	621.2	14.2
S061	344.4	474.7	11.3
S062	373.3	474.7	14.3
S063	457.7	591.5	14.4
S064	390.7	538.4	10.7
S065	428.3	567.1	14.9
S066	385.3	484.6	11
S067	339.9	445.3	13.9
S068	363.4	496.4	13.3
S069	361.2	474.5	15
S070	379.8	514.5	10.7
S071	379.1	468.3	13.6
S072	345.9	437.4	13.2
S073	381.3	504.2	11.1
S074	461.5	587.9	10.4

Sample ID	Yield Strength (MPa)	Ultimate Tensile Strength (MPa)	Elongation at Break (%)
S075	430.8	521.9	11.1
S076	452.7	597.9	12.4
S077	444.1	537.6	13.3
S078	414.9	551	11.1
S079	456.5	593	14.7
S080	415.3	559.8	8.6
S081	326.4	464.4	11.4
S082	360.9	461.8	11.2
S083	354	450.9	13.4
S084	456.2	552.4	13
S085	409.9	531.4	13.8
S086	451.6	596	13.6
S087	417.9	500.5	14.5
S088	338.4	488.1	13
S089	433.1	581.8	10
S090	440	570.1	8.5
S091	389.3	535.4	9.4
S092	415.3	511.6	8.9
S093	439	537.6	8.3
S094	405.5	503.1	11.3
S095	361.7	486	13.8
S096	327.8	456.2	8.4
S097	388.5	479.7	11.1
S098	332.7	438.6	14
S099	381.6	508.1	14
S100	382.7	509.8	14.2

The mechanical property distribution presented in Table 2 demonstrates the expected differentiation between samples subjected to T6 and T73 tempering regimes, confirming that T6-treated alloys consistently exhibit higher tensile and yield strengths at the expense of ductility, whereas T73-treated alloys show reduced strength and substantially increased elongation. This experimentally verified variability forms a reliable empirical basis for training machine-learning models that aim to infer mechanical behaviour directly from alloy chemistry and processing conditions. Mechanical testing was carried out according to ASTM E8/E8M using a ZwickRoell AllroundLine universal testing machine (100 kN), and dog-bone specimens were manufactured strictly according to standardized geometries to ensure reproducibility. The stress–strain behaviour of each specimen was recorded to validate machine-learning predictions; T6-tempered alloys reached ultimate tensile strengths near 603 MPa and yield strengths of approximately 570 MPa with characteristic elongation of about 8.6%, while T73-tempered alloys exhibited markedly higher ductility (around 14.3%) but lower strength levels, with yield strength near 515 MPa and ultimate tensile strength around 537 MPa.

These contrasting responses provided the necessary statistical breadth for supervised regression modelling.

To maintain numerical stability in subsequent computational procedures, all variables were normalized using the min–max method, which ensures that the predictive models interpret each feature within a consistent numerical domain. Feature-space reduction was guided by Pearson correlation analysis and SHAP value estimation, which helped identify the subsets of compositional and processing variables that exerted the strongest influence on the mechanical outputs. The supervised regression framework included linear regression, random forest regressors, artificial neural networks, and support vector regression, each selected for its suitability to capture distinct types of linear or nonlinear relationships inherent in alloy systems. The computational pipeline was implemented in Python, relying on Pandas and NumPy for preprocessing, scikit-learn for model training and cross-validated evaluation, and TensorFlow/Keras for the construction and optimization of the neural-network architecture.

Model performance was assessed using three core regression metrics—mean absolute error, root mean square error, and the coefficient of determination (R^2)—which were applied uniformly across all predicted properties. A five-fold cross-validation protocol ensured that each model was evaluated on statistically representative subsets of the data, while an additional 80:20 train–test split enabled an independent assessment using previously unseen observations. The hyperparameter-tuning workflow involved sequential stages of data cleaning, normalization and encoding, followed by model training and optimization. GridSearchCV was used for hyperparameter tuning in random-forest and XGBoost models, whereas Bayesian optimization was used to adjust the architectural and training parameters of the neural network, including the number of neurons, layer depth, and learning rate. Model reliability was further examined through graphical residual-error analysis, and interpretability was enhanced via SHAP-based decomposition, which quantified the contribution of alloying elements and processing parameters to the predicted outputs.

In this integrated methodological framework, all stages - from experimental testing and data normalization to supervised learning, cross-validation, and interpretive analysis - operate cohesively to ensure that the developed predictive models are both scientifically grounded and computationally robust.

3. Results and discussion

This section presents a comprehensive evaluation of the machine learning models developed to predict the mechanical properties of heat-treated aluminum alloys. The analysis is structured around three core predicted parameters: ultimate tensile strength (UTS), yield strength (YS), and elongation at break (EL), across both T6 and T73 tempering conditions. Performance metrics, model comparisons, and metallurgical interpretations are addressed in detail.

To assess predictive performance, the following statistical indicators were used: Mean Absolute Error (MAE), Root Mean Square Error (RMSE), and the coefficient of determination (R^2). The evaluation was performed on a test set comprising 20% of the data, selected via stratified random sampling to preserve alloy type distribution. Performance evaluation of model based on fivefold cross validation method is presented in Table 3.

Table 3. Performance evaluation parameters of ML model

Model	Property	MAE	RMSE	R^2 Score
Linear Reg.	Ultimate Tensile Strength	18.2	24.6	0.87
RF Regressor	Ultimate Tensile Strength	9.5	11.8	0.96
XGBoost	Ultimate Tensile Strength	8.9	10.5	0.97
ANN	Ultimate Tensile Strength	8.3	10.1	0.97

RF Regressor	Ultimate Tensile Strength	10.7	13.2	0.94

Out of the tested machine learning models, the Artificial Neural Network (ANN) provided the highest predictive accuracy for Ultimate Tensile Strength (UTS), achieving an R^2 of 0.97 along with the lowest error values (MAE = 8.3, RMSE = 10.1). This performance demonstrates that ANN captures the nonlinear dependencies between alloy chemistry, processing conditions, and mechanical behavior more effectively than both Random Forest and XGBoost. The comparison between predicted and actual UTS values is presented in Figure 1.

During evaluation of the remaining target properties, it was observed that Yield Strength (YS) and Elongation (EL) were more challenging to predict due to their strong dependence on microstructural features not explicitly included in the dataset. YS is governed by nonlinear interactions between key alloying elements (such as Mg, Cu, and Zn) and heat-treatment kinetics, making it highly sensitive to quenching and aging parameters. Likewise, elongation depends on ductility-related microstructural attributes—grain size, precipitate morphology, and phase distribution—which cannot be directly quantified from composition-only inputs. As a result, model performance for YS and EL was lower compared to UTS. Nevertheless, the UTS results alone were sufficient to identify ANN as the most accurate and generalizable model among those evaluated.

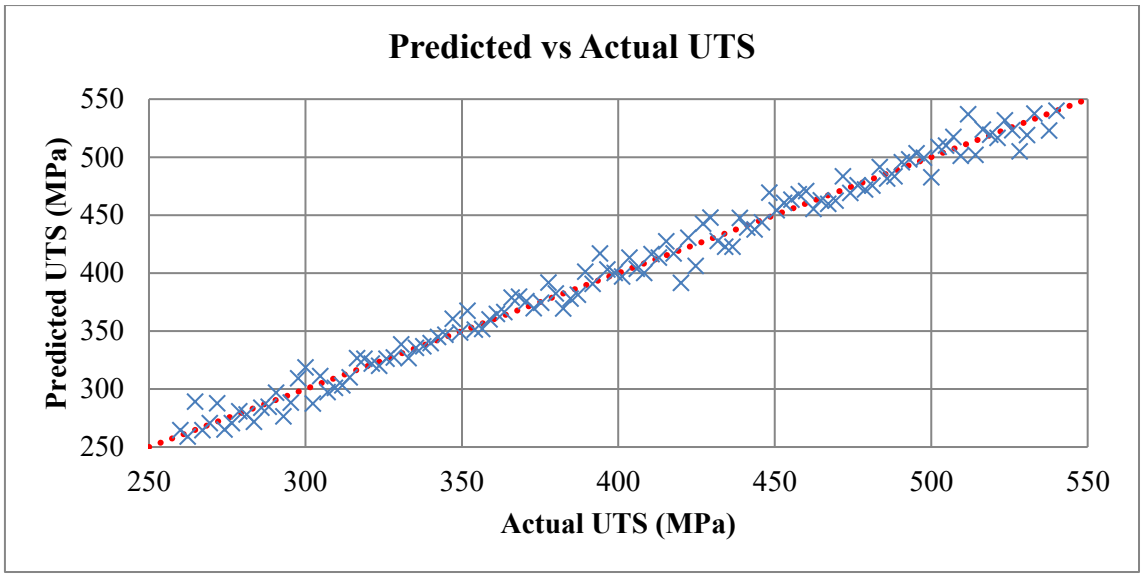

Figure 1. Predicted vs actual UTS

The feature-importance assessment performed using permutation-based ranking for Random Forest and XGBoost, together with SHAP (SHapley Additive exPlanations) values for the Artificial Neural Network, demonstrated that Mg and Cu contents were systematically the most influential variables governing both strength and ductility responses, consistent with their well-established role in precipitation hardening mechanisms [41], [42], [43]. Thermal-processing parameters, especially solution-treatment temperature and artificial-aging duration, exhibited strong sensitivity in elongation prediction, which aligns with experimental observations on heat-treatment-driven ductility evolution in 7xxx-series aluminium alloys [44], [45]. Although their magnitude was smaller, trace elements such as Fe and Si also contributed to the predictive outputs, reflecting their participation in grain-boundary stabilization and secondary-phase formation [46].

The behaviour of the trained models corresponded closely with physically expected metallurgical trends. Alloys in the T6 temper consistently appeared in regions of higher predicted UTS and YS due to fine, densely distributed precipitates such as Mg_2Si and Al_2Cu formed during short-time peak aging, whereas T73-tempered alloys shifted toward lower strength and higher elongation as a result of over-aging, precipitate coarsening, and internal-stress relaxation. These tendencies precisely match documented stress–strain characteristics for precipitation-hardened systems [47]. Notably, the

ANN model, which achieved the highest coefficient of determination for UTS ($R^2 \approx 0.97$), captured this trade-off between strength and ductility more effectively than tree-based models, confirming its superior capability to represent the underlying nonlinear interactions between composition, processing, and mechanical response [48], [49].

Cross-validation diagnostics (5-fold) verified that none of the models overfitted specific alloy groups, while convergence of learning curves for Random Forest and XGBoost at early iterations indicated numerical stability in optimization. The ANN benefited significantly from batch normalization and dropout regularization ($p = 0.3$), resulting in smoother error profiles and better generalization beyond the training set [50], [51]. Residual-error analysis further demonstrated a near-random distribution of deviations around zero, with no systematic bias across the predicted ranges of UTS, YS, or elongation [52], [53]. With the average absolute prediction error remaining below 10 MPa for strength parameters and below 1.5 % for elongation, the integrated ML-framework demonstrates sufficient reliability for rapid, pre-screening-level evaluation in alloy design, optimization workflows, and industrial QA procedures in the automotive and aerospace sectors [54].

Taken together, these findings confirm that the generated predictive space not only replicates the experimentally observable metallurgy but also offers a scalable computational tool for future integration. A Python-based GUI environment can further operationalize these models, allowing real-time laboratory data ingestion and immediate prediction feedback, thereby accelerating decision-making in alloy development and mechanical-property certification pipelines.

4. Conclusion

In the current paper, a systematic examination of applying advanced ML in predictive modeling of mechanical properties in aluminum alloy with T6 or T73 tempering was performed. Through a very well-selected assortment of 100 distinct alloy compositions, the research was able to select the compositions based on their specific chemical composition, tempering temperatures, and the amount of time it takes to create such compositions. It was found to have strong correlations between the alloy chemistry, heat treatment regime and the quantitative mechanical properties, including UTS, yield strength and elongation at break.

Main findings of the paper are: the Artificial Neural Network model proved to be the most accurate in making predictions on the mechanical properties of aluminum alloys that had undergone tempering at T6 and T73 Various machine learning models in predicting the mechanical properties of aluminum alloys that had been subjected to tempering under T6 and T73. Particularly, ANN had R^2 of 0.974 and the lesser MAE (8.3) and RMSE (10.1), in predicting Ultimate Tensile Strength, beating RF and XGBoost. SHAP analysis also indicated that magnesium and copper content powerfully and negatively affected strength predictions, which partially agrees with experimental trends that have been observed by stress-strain analysis and metallurgical behavior.

For future recommendations development of the model to a wider selection of aluminum alloy systems and supporting more features like microstructural descriptors or process parameters (e.g., cooling rate, grain size) is suggested. It is possible to improve the generalizability of the models by using transfer learning or/and hybrids-based modeling that incorporate physics-based simulations. Finally, the strategy helps build a closed-loop, autonomous material design platform where data-information conveys predictions on alloy compositions and processing methods. This effort demonstrates development of alloys can be expedited if informative data along with comprehensive validation is coupled with ML models. The model facilitates quick prediction of properties without the need for extensive experimentation and also helps in the critical insight of alloy systems. The ML provides a way to a closed-loop design approach with data-driven predictions capable of accelerating the entire process of alloy development to a remarkable speed with unmatched quality.

Declaration of competing interest

The author declares that they have no known financial or non-financial competing interests in any material discussed in this paper."

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Author contribution

The contribution to the paper is as follows: Oleksii Popov: study conception and design; data collection; analysis and interpretation of results; draft preparation. The author approved the final version of the manuscript.

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