HARDNESS PREDICTION OF AlxCoCrFeMnNi HEA VIA INTERPOLATION FUNCTION

PREVISÃO DA DUREZA DA LIGA DE ALTO-HEA AlxCoCrFeMnNi VIA FUNÇÃO DE INTERPOLAÇÃO

PREDICCIÓN DE LA DUREZA DE AL[A]X[CoCrFeMnNi] HEA MEDIANTE FUNCIÓN DE INTERPOLACIÓN

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ABSTRACT

High-entropy alloys (HEAs) are eminent in materials engineering in view of the vast universe of possible combination of elements. This addresses diversity in properties, which demands prediction to prevent unnecessary experiments. Therefore, this work presents an interpolation scheme of Vickers' hardness in terms of the composition of aluminum in $Al_xCoCrFeMnNi$ (x = 0.1 to 1) HEA. Initial data from literature were the basis to develop the polynomials from first to ninth degree. These polynomials were compared to check which one gives the minimum relative percentage error to be elected as a possible predictor of Vickers' hardness of this HEA as a function of aluminum composition. As a result, the proposed interpolation function turned out to be a mixed solution between the 6th.-, 7th.-, and 9th.-degree polynomials, which presented a maximum relative percentage error of 4.51%, allowing the proposed mathematical model to predict Vickers' hardness of this alloy within the referred range of composition.

Keywords: Hardness. Prediction. High-Entropy Alloys. Interpolation Function. Alloy.

RESUMO

As ligas de alta entropia (HEAs) são de grande importância na engenharia de materiais devido ao vasto universo de combinações possíveis de elementos. Isso resulta em diversidade de propriedades, o que exige previsão para evitar experimentos desnecessários. Portanto, este trabalho apresenta um esquema de interpolação da dureza Vickers em função da composição de alumínio na HEA $AlxCoCrFeMnNi$ (x = 0,1 a 1). Dados iniciais da literatura serviram de base para o desenvolvimento de polinômios do primeiro ao nono grau. Esses polinômios foram comparados para verificar qual deles apresenta o menor erro percentual relativo para ser escolhido como possível preditor da dureza Vickers dessa HEA em função da composição de alumínio. Como resultado, a função de interpolação proposta mostrou ser uma solução mista entre os polinômios de 6º, 7º e 9º graus, que apresentou um erro

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percentual relativo máximo de 4,51%, permitindo que o modelo matemático proposto preveja a dureza Vickers dessa liga dentro da faixa de composição considerada.

Palavras-chave: Dureza. Previsão. Ligas de Alta Entropia. Função de Interpolação. Liga.

RESUMEN

Las aleaciones de alta entropía (HEA) son fundamentales en la ingeniería de materiales debido al amplio universo de posibles combinaciones de elementos. Esto aborda la diversidad de propiedades, lo que exige predicciones para evitar experimentos innecesarios. Por lo tanto, este trabajo presenta un esquema de interpolación de la dureza Vickers en función de la composición de aluminio en las HEA *AlxCoCrFeMnNi (x* = 0,1 a 1). Los datos iniciales de la literatura sirvieron de base para desarrollar los polinomios de primero a noveno grado. Estos polinomios se compararon para comprobar cuál presentaba el mínimo error porcentual relativo para ser elegido como posible predictor de la dureza Vickers de esta HEA en función de la composición del aluminio. Como resultado, la función de interpolación propuesta resultó ser una solución mixta entre los polinomios de sexto, séptimo y noveno grado, que presentó un error porcentual relativo máximo del 4,51 %, lo que permitió al modelo matemático propuesto predecir la dureza Vickers de esta aleación dentro del rango de composición mencionado.

Palabras clave: Dureza. Predicción. Aleaciones de Alta Entropía. Función de Interpolación. Aleación.

1 INTRODUCTION

The enhancement of materials properties has been object of research and development throughout the centuries. Although the state of the art in this area corresponds to a robust body of knowledge, the potential of developing new solutions is significant. The branches of development include the improvement of existing materials and the creation of others (NONATO *et al*., 2025).

Consequently, since the improvement of mechanical properties is one of the main drivers of materials area, it turns out to be a technical concern (CALLISTER JUNIOR; RETHWISCH, 2020). Related to metallic materials, alloys play one of the most important roles in the improvement of mechanical properties. Two-element alloys have significantly enhanced the properties of materials, but they present limitations in terms of magnitude (RAZUAN *et al*., 2013).

The issue related to the threshold of two-component alloys led to the development of multicomponent alloys (MAs) (CANTOR *et al*., 2004) (YEH *et al*., 2004) (RESTIVO; RESTIVO, 2021), which consists of three or more main elements. These alloys offer a great variety of compositions in terms of combinatorial analysis, although some combinations should be physically examined to investigate their feasibility. Therefore, the number of elements, their nature, molar fraction, and manufacturing route determine the mechanical properties of the alloy (RESTIVO *et al*., 2023).

The high number of possible combinations of MAs turns the trial-and-error approach infeasible. In view of this, the microstructure as well as the magnitudes of the properties should be predicted/simulated. The prediction intends to prevent unnecessary experimentation that may result in non-desired magnitudes of properties and/or types of microstructures. The configurational entropy of MAs determines their categorization as the following: (a) low-entropy alloys (LEAs); (b) medium-entropy alloys (MEAs); and (c) high-entropy alloys (HEAs) (NONATO; RESTIVO, 2024). The higher number of constituting elements leads to a higher configurational entropy.

Commonly, 5 to 13 main elements (5 to 35% in molar fraction of each element) compose HEAs, as well as minor elements (molar fraction of each element lower than 5%). More elements to combine addresses wider ranges of properties, which could be more difficult to predict. Furthermore, high entropy in solidification process may induce solid solutions, which could be advantageous to practical applications.

2 OBJECTIVE

The main objective is to obtain an interpolation function to predict Vickers' hardness of $Al_xCoCrFeMnNi$ (x = 0.1 to 1) alloy within the range of composition of aluminum, which in molar fraction goes from 1.96 to 16.67%.

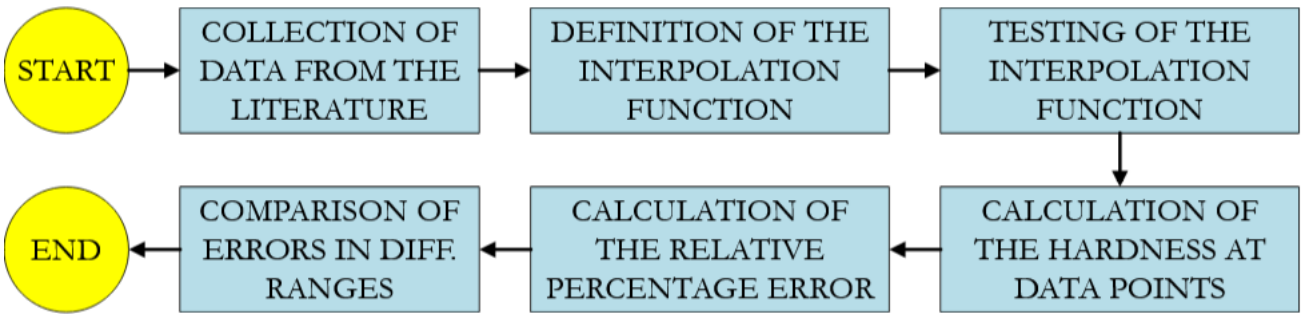
3 METHODOLOGY

The methodology adopted in this work is summarized in the flowchart in Figure 1. The upper line of the flowchart is described as follows: the data related to Vickers' hardness for certain compositions were extracted from the literature. All data were used to construct the interpolation functions (from first-degree polynomial to ninth-degree polynomial), thus generating the corresponding numbers of coefficients, and Vickers' hardness values. The testing of all interpolation functions was performed to analyze their feasibility.

The lower line of the flowchart refers to the calculation of the hardness at data points (which can be taken from the previous step) to calculate the relative percentage error at each point. Thenceforth, the comparison of errors in different ranges of the domain is accomplished to determine which interval is more reliable.

Figure 1

Flowchart of the steps of this paper.



Source: Own authorship, 2026.

4 DEVELOPMENT

This section shows the development of the methodology described in Figure 1. Values of Vickers' hardness were extracted from (BORG *et al*., 2020) for $Al_xCoCrFeMnNi$ (x = 0.1 to 1). According to Table 1, the range of variation of aluminum content in molar fraction goes from 1.96 to 16.67%, while the molar fraction of any other element in the composition ranges from 16.67 to 19.61% (which corresponds to a range in hardness from 180 to 684 HV).

Table 1

Molar fraction of the 6 elements in each HEA, and hardness of the 13 HEAs.

HEA number	HEA	Molar fraction of Al (%)	Molar fraction of any other element (%)	Hardness (HV)
1	Al0.1CoCrFeMnNi	1.96	19.61	180
2	Al0.2CoCrFeMnNi	3.85	19.23	171
3	Al0.38CoCrFeMnNi	7.06	18.59	182
4	Al0.43CoCrFeMnNi	7.92	18.42	183
5	Al0.49CoCrFeMnNi	8.93	18.21	220
6	Al0.56CoCrFeMnNi	10.07	17.99	278
7	Al0.62CoCrFeMnNi	11.03	17.79	405
8	Al0.68CoCrFeMnNi	11.97	17.61	486
9	Al0.75CoCrFeMnNi	13.04	17.39	530
10	Al0.81CoCrFeMnNi	13.94	17.21	539
11	Al0.88CoCrFeMnNi	14.97	17.01	533
12	Al0.95CoCrFeMnNi	15.97	16.81	535
13	AlCoCrFeMnNi	16.67	16.67	684

Source: own authorship (2026).

Based on the available data, all HEAs were applied to build up the interpolation functions in the software Matlab®. Nine degrees of polynomials were used to predict hardness of the alloys (from 1st. to 9th.). Table 2 presents the calculated coefficients of the polynomials, in which, for example, the 1st.-degree polynomial corresponds to Equation 1, and the 4th.-degree polynomial refers to Equation 2, where x is the aluminum content (as per $Al_xCoCrFeMnNi$ (x = 0.1 to 1)), and HV_n is the Vickers' hardness based on the n-th-degree polynomial.

$$HV_1(x) = 605.20\,x + 13.46. \quad (1)$$

$$HV_4(x) = 1840\,x^4 + 6355\,x^3 + 7266\,x^2 + 2514\,x + 386.80. \quad (2)$$

Table 2

Polynomials coefficients.

Order of the coefficient	1st.-dp	2nd.-dp	3rd.-dp	4th.-dp	5th.-dp	6th.-dp	7th.-dp	8th.-dp	9th.-dp
0th.	13.46	126.90	317.50	386.80	-217	503.50	1034	2549	11060
1st.	605.20	81.93	1633	2514	7206	-7115	-18980	-55660	296600
2nd.	0.00	464	4159	7266	42360	56060	152800	490000	-3090000
3rd.	0.00	0.00	2228	6355	102500	208800	593300	2177000	17080000
4th.	0.00	0.00	0.00	1840	105000	389800	1218000	5473000	-56190000
5th.	0.00	0.00	0.00	0.00	38600	345700	1333000	8155000	115500000
6th.	0.00	0.00	0.00	0.00	0.00	116000	728700	7178000	149900000
7th.	0.00	0.00	0.00	0.00	0.00	0.00	-154500	3473000	119200000
8th.	0.00	0.00	0.00	0.00	0.00	0.00	0.00	716400	-53090000
9th.	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	10140000

Source: own authorship (2026).

Table 3 shows hardness values for each HEA (row) and for each polynomial degree (column), which corresponds to the calculation of the hardness at data points, such that each row (from second on) corresponds to each HEA and each column refers to the degree of the interpolation polynomial. The accuracy of prediction via the obtained interpolation functions in terms of the relative percentage error is presented in Table 4. Negative values indicate that the calculated value is lower than the those experimentally obtained, while positive values refer to calculated values higher than the experimental.

Table 3

Hardness values (in HV) for each degree, in which dp stands for degree polynomial.

HEA number	1st.-dp	2nd.-dp	3rd.-dp	4th.-dp	5th.-dp	6th.-dp	7th.-dp	8th.-dp	9th.-dp
1	73.99	139.71	193.49	201.85	172.39	179.46	179.95	180.05	180.00
2	134.51	161.83	139.33	126.73	193.90	173.02	171.18	170.70	171.03
3	243.45	225.02	175.13	170.40	142.93	174.79	181.99	186.21	180.06
4	273.71	247.91	207.03	206.98	172. 74	184.72	182.79	178.69	189.75
5	310.02	278.43	253.64	258.03	233.94	220.95	214.25	210.97	208.89
6	352.39	318.27	315.87	322.65	325.54	299.51	296.73	299.70	290.53
7	388.70	356.04	372.64	378.68	404.61	387.14	390.52	394.13	396.74
8	425.01	397.15	429.51	432.53	469.49	472.88	478.69	477.73	486.83
9	467.38	449.33	492.16	489.91	515.28	539.62	540.57	536.15	532.84
10	503.69	497.68	539.37	532.81	528.61	550.63	545.37	545.24	536.67
11	546.06	558.31	582.84	574.40	532.21	522.28	518.50	523.92	533.80
12	588.42	623.49	609.43	606.66	570.18	536.44	543.90	539.65	534.83
13	618.68	672.82	615.55	624.38	664.19	684.57	681.56	682.85	684.02

Source: own authorship (2026).

Table 4

Relative percentage error between calculated and experimental hardnesses.

HEA number	1st.-dp Re (%)	2nd.-dp Re (%)	3rd.-dp Re (%)	4th.-dp Re (%)	5th.-dp Re (%)	6th.-dp Re (%)	7th.-dp Re (%)	8th.-dp Re (%)	9th.-dp Re (%)
1	-58.90	-22.38	7.49	12.14	-4.23	-0.30	-0.03	0.03	0.01
2	-21.34	-5.36	-18.52	-25.89	13.39	1.18	0.11	-0.17	0.02
3	33.76	23.64	-3.78	-6.38	-21.47	-3.96	-0.01	2.32	-1.06
4	49.57	35.47	13.13	13.10	-5.61	0.94	-0.12	-2.35	3.69
5	40.92	26.56	15.29	17.29	6.34	0.43	-2.61	-4.10	-5.05
6	26.76	14.49	13.62	16.06	17.10	7.74	6.74	7.81	4.51
7	-4.02	-12.09	-7.99	-6.50	-0.10	-4.41	-3.58	-2.68	-2.04
8	-12.55	-18.28	-11.62	-11.00	-3.40	-2.70	-1.50	-1.70	0.17
9	-11.82	-15.22	-7.14	-7.56	-2.78	1.82	1.99	1.16	0.54
10	-6.55	-7.67	0.07	-1.15	-1.93	2.16	1.18	1.16	-0.43
11	2.45	4.75	9.35	7.77	-0.15	-2.01	-2.72	-1.70	0.15
12	9.99	16.54	13.91	13.39	6.58	0.27	1.66	0.87	-0.03
13	-9.55	-1.63	-10.01	-8.72	-2.90	0.08	-0.36	-0.17	0.01

Source: own authorship (2026).

The observation of Table 4 addresses impractical relative percentage errors from 1st.-degree to 5th.-degree polynomial. In view of this, just 6th. to 9th. range of relative percentage errors are analyzed aiming at minimizing the error. For the first two HEAs, the 9th.-degree

polynomial presents the lowest value of error; HEAs 3 and 4 hardness values are better represented by 7th.-degree polynomial; 6th.-degree polynomial better represents HEA 5; From HEA 6 to 13, 9th.-degree polynomial presents the lowest relative percentage error. Therefore, Equation 3, Equation 4, and Equation 5 are those applied in the prediction of hardness values as the aluminum content varies from *x* = 0.1 to 1.

$$HV_6(x) = 116000\,x^6 + 345700\,x^5 + 389800\,x^4 + 208800\,x^3 + 56060\,x^2 - 7115\,x + 503.50. \quad (3)$$

$$HV_7(x) = -154500\,x^7 + 728700\,x^6 + 1333000\,x^5 + 1218000\,x^4 + 593300\,x^3 + 152800\,x^2 - 18980\,x + 1034. \quad (4)$$

$$HV_9(x) = 10140000\,x^9 - 53090000\,x^8 + 119200000\,x^7 + 149900000\,x^6 + 115500000\,x^5 - 56190000\,x^4 + 17080000\,x^3 - 3090000\,x^2 + 296600\,x + 11060. \quad (5)$$

Thenceforth, the final expression that represents the model that minimizes the relative error is given by Equation 6, where four intervals are defined within the range $0.1 \leq x \leq 1$.

$$HV(x) = \begin{cases} HV_9(x)\ for\ 0.1 \leq x < 0.29 \wedge 0.525 < x \leq 1 \\ HV_7(x)\ for\ 0.29 \leq x < 0.46 \\ HV_6(x)\ for\ 0.46 \leq x \leq 0.525 \end{cases} \quad (6)$$

5 FINAL CONSIDERATIONS

In this paper, *Al$_x$CoCrFeMnNi* (*x* = 0.1 to 1) HEAs were investigated in terms of Vickers' hardness. Thirteen different compositions associated with their hardness values were extracted from the literature and subjected to an algorithm that extracts the interpolations functions (from first-degree to ninth-degree polynomials).

The resulting polynomial reflects a mixed solution between the 6th.-, 7th.-, and the 9th-degree polynomials. This yields minimum and maximum relative percentage errors of 0.01 and 4.51%, respectively. Therefore, the interpolation function proposed herein may be used to predict Vickers' hardness of *Al$_x$CoCrFeMnNi* (*x* = 0.1 to 1), which may avoid expensive experiments, observing the maximum relative percentage error reported.

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