RELATIONSHIP BETWEEN POLYDISPERSION OF ATOMIC RADII AND HARDNESS IN HIGH-ENTROPY ALLOYS

RELAÇÃO ENTRE A POLIDISPERSÃO DE RAIOS ATÔMICOS E A DUREZA EM LIGAS DE ALTA ENTROPIA

RELACIÓN ENTRE LA POLIDISPERSIÓN DE RADIOS ATÓMICOS Y LA DUREZA EN ALEACIONES DE ALTA ENTROPÍA

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ABSTRACT

High-entropy alloys (HEAs) are one of the most important discoveries regarding metallic materials in this century. HEAs have become a breakthrough related to binary and ternary alloys in terms of microstructure and properties. The vastness of possible combinations of elements addresses complexity and demands investment to obtain the required properties via experiments. To overcome this drawback, the efforts have increasingly been directed to the prediction of the properties, thus minimizing, or even preventing experiments. Therefore, in the context of HEAs, this paper focuses on obtaining the relationship between hardness and polydispersion of atomic radii, which is one of the parameters studied in topological parameters calculation approach (TPC). Data on thirty HEAs were collected from the literature, from which the hardness was extracted, the calculation of the topological discrepancy was accomplished, and the relationship between polydispersion of atomic radii and hardness was established. The results showed that the relationship between hardness and polydispersion of atomic radii has low correlation, and, therefore, it is difficult to build an interpolation polynomial to predict values of hardness without incurring in high levels of error.

Keywords: Hardness. Prediction. High-Entropy Alloys. Polydispersion of Atomic Radii. Alloy.

RESUMO

As ligas de alta entropia (HEAs) representam uma das descobertas mais importantes em relação aos materiais metálicos neste século. As HEAs constituíram um avanço significativo em relação às ligas binárias e ternárias em termos de microestrutura e propriedades. A vasta gama de combinações possíveis de elementos implica complexidade e demanda investimento para a obtenção das propriedades desejadas por meio de experimentos. Para superar essa desvantagem, os esforços têm sido cada vez mais direcionados à predição das propriedades, minimizando, ou mesmo dispensando, a necessidade de experimentos. Portanto, no contexto das HEAs, este artigo concentra-se na obtenção da relação entre

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dureza e polidispersão dos raios atômicos, um dos parâmetros estudados na abordagem de cálculo de parâmetros topológicos (TPC). Dados de trinta HEAs foram coletados da literatura, dos quais a dureza foi extraída, o cálculo da discrepância topológica foi realizado e a relação entre a polidispersão dos raios atômicos e a dureza foi estabelecida. Os resultados mostraram que a relação entre dureza e polidispersão dos raios atômicos apresenta baixa correlação e, portanto, é difícil construir um polinômio de interpolação para prever valores de dureza sem incorrer em altos níveis de erro.

Palavras-chave: Dureza. Predição. Ligas de Alta Entropia. Polidispersão de Raios Atômicos. Liga.

RESUMEN

Las aleaciones de alta entropía (HEA) constituyen uno de los descubrimientos más importantes en el campo de los materiales metálicos en este siglo. Han supuesto un gran avance en el campo de las aleaciones binarias y ternarias en términos de microestructura y propiedades. La amplia gama de combinaciones posibles de elementos plantea una gran complejidad y exige inversión para obtener las propiedades requeridas mediante experimentos. Para superar esta desventaja, los esfuerzos se han dirigido cada vez más a la predicción de las propiedades, minimizando o incluso eliminando los experimentos. Por lo tanto, en el contexto de las HEA, este artículo se centra en la obtención de la relación entre la dureza y la polidispersión de los radios atómicos, que es uno de los parámetros estudiados en el enfoque de cálculo de parámetros topológicos (CPT). Se recopilaron datos de treinta HEA de la literatura, de los cuales se extrajo la dureza, se realizó el cálculo de la discrepancia topológica y se estableció la relación entre la polidispersión de los radios atómicos y la dureza. Los resultados mostraron que la relación entre la dureza y la polidispersión de los radios atómicos presenta una baja correlación y, por lo tanto, resulta difícil construir un polinomio de interpolación para predecir valores de dureza sin incurrir en altos niveles de error.

Palabras clave: Dureza. Predicción. Aleaciones de Alta Entropía. Polidispersión de Radios Atómicos. Aleación.

1 INTRODUCTION

The progress of our society is frequently associated with the evolution of technology. In materials area, the capability to accomplish increasingly challenging tasks was dictated by the capacity to improve material properties, which has been an ever-growing demand throughout the ages (NONATO *et al*., 2025). The established body of knowledge associated with findings in this area speeded up the development of new materials to fulfill some of the existing requirements. However, there is still a gap between the requirements and the current available solutions.

In materials design, the mechanical properties are the main drivers of the research and development branch, leading to a great number of experiments to validate the enhancement of an existing material or even the creation of a new one. In other words, the material is tailored aiming at reaching planned ranges of properties (CALLISTER JUNIOR and RETHWISCH, 2020).

In view of this, the nature of the elements involved, their proportion, and the manufacturing route impacts the microstructure, which affects the mechanical properties (RESTIVO *et al*., 2023). In the branch of metallic materials, one or more metals and/or non-metals are combined to form the so-called alloys. A previous alternative was the pure metals, but the limitations are well known, according to the applications (RAZUAN *et al*., 2013). Therefore, metal alloys are designed to widen the ranges of properties, allowing the new possibilities and/or applications. Metal alloys can be classified as conventional (when there are two main elements, being metals or non-metals) (SHUN *et al*., 2012). Examples of the most found properties in the literature are: (a) density; (b) ductility; (c) tenacity; (d) fracture toughness; (e) Young's modulus; (f) thermal stability; (g) hardness; among others.

Although the information is more abundant in the case of conventional alloys (phase diagrams, experiments, manufacturing routes, etc.), the limitations in terms of ranges of properties restrict their application (RESTIVO; RESTIVO, 2021). The enhancement of the properties of an alloy can be achieved by combining more elements into the concept of a multicomponent alloy (MA). An MA consists of three or more main elements that may enhance the performance in existing applications, and/or enable new ones. The main classification of MAs refers to configurational entropy: (a) low-entropy alloys (LEAs); (b) medium-entropy alloys (MEAs); and (c) high-entropy alloys (HEAs) (NONATO; RESTIVO, 2024).

In the manufacturing process of MAs complex microstructures associated with undesired ranges of properties may be achieved. These unplanned results may be minimized using prediction techniques, which aid in the tailoring of the properties of the material even

before its manufacturing. Simulation and/or calculation may be used to predict microstructures as well as properties in order to avoid or diminish the necessity of experimentation.

2 OBJECTIVE

The main objective is to obtain the relationship between hardness and polydispersion of atomic radii based on hardness data of thirty different equimolar HEAs, and their calculated polydispersion of atomic radii.

3 METHODOLOGY

The strategy applied in this work addresses the sequence of steps represented in Figure 1. The methodology covers the following steps:

(a) Gathering data from the literature: data of hardness for thirty HEAs were extracted from the reference (BORG *et al.*, 2020).

(b) Calculation of the molar fraction of each element: since all HEAs presented here are equimolar, with 5-, and 6-element HEAs, the molar fractions are, respectively, 1/5 and 1/6.

(c) Calculation of the mean radius of the alloy, r_m: it is the weighted mean of the atomic radii of the elements involved, as per Equation 1, where n is the number of elements of the alloy, f_i is the molar fraction of the i-th element, and r_i is the radius of the i-th element of the alloy:

$$r_m = \sum_{i=1}^{n} f_i \, r_i. \qquad (1)$$

(d) Calculation of the polydispersion of atomic radii (δ): it is the mean square deviation resulting from the atomic radii of the elements involved, as per Equation 2:

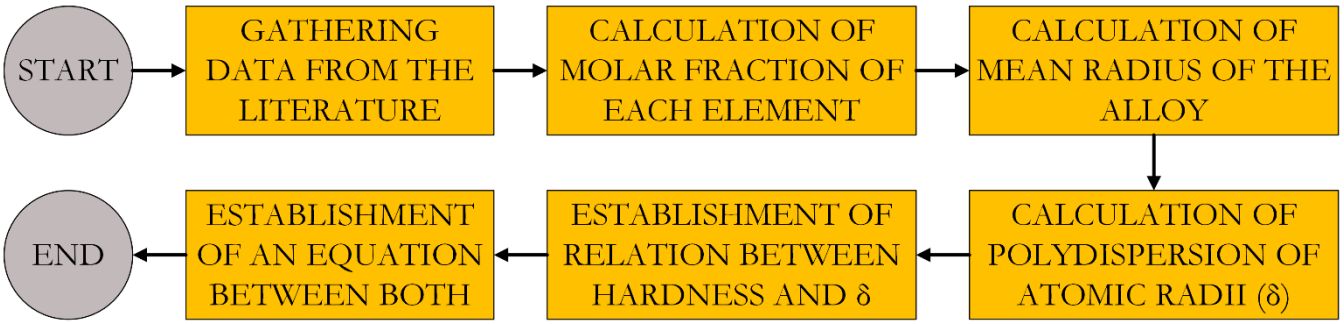
$$\delta = \sqrt{\sum_{i=1}^{n} f_i \left(\frac{1-r_i}{r_m}\right)^2}. \qquad (2)$$

(e) Establishment of the relation between hardness and δ: refers to the behavior of hardness (in Vickers) and the polydispersion of atomic radii.

(f) Establishment of an equation between both: creation of an equation that maps hardness (in Vickers) related to δ.

Figure 1

Flowchart of the steps of this paper.



Source: Own authorship, 2026.

4 DEVELOPMENT

This section presents the development of the methodology shown in the previous section. The thirty HEAs were listed in the second column of Table 1, and each HEA is associated with a number at the first column. Since all HEAs in this paper are equimolar, the molar fraction of each constitutive element is equal, a simple division of the representativeness of the element by the number of elements yieldsthe results in the third column. In addition, the fourth column represents Vickers' hardness of each HEA, which were extracted from (BORG *et al*., 2020).

Table 1

Thirty HEAs, the molar fraction of each element, and the hardness of the alloy.

HEA number	HEA	Molar fraction of each element	Hardness (HV)
1	AlHfNbTaTiZr	1/6	441.00
2	AlMoNbTiV	1/5	537.00
3	CrNbTiVZr	1/5	482.00
4	HfMoNbTaTiZr	1/6	505.00
5	HfMoTaTiZr	1/5	542.00
6	MoNbTaVW	1/5	536.00
7	AlCoCrCuFeNi	1/6	472.00
8	AlCoCuFeNi	1/5	536.00
9	AlCoCuFeNiTi	1/6	626.00
10	AlCoCuFeNiZr	1/6	472.00
11	CoCuFeMnNi	1/5	208.00
12	AlCrCuFeNi	1/5	495.00
13	CoCrCuFeNi	1/5	286.00
14	AlCuFeNiTi	1/5	516.00
15	CoFeMoNiV	1/5	625.00
16	HfNbTaTiZr	1/5	420.00
17	MoNbTaTiW	1/5	507.50
18	CoCrFeMnNi	1/5	130.20
19	AlCoCrFeMnNi	1/6	684.00
20	CrMoNbTaVW	1/6	1072.00
21	CoCrCuFeNi	1/5	286.00
22	CrCuFeMnNi	1/5	296.00
23	CrCuFeMoNi	1/5	263.00

24	AlFeNiTiVZr	1/6	800.00
25	AlCoCrFeNi	1/5	484.00
26	AlCoCrCuFe	1/5	407.00
27	CuFeNiTiVZr	1/6	590.00
28	FeMoNiTiVZr	1/6	740.00
29	CoCrFeMnNiV	1/6	636.00
30	AlCrFeMoNi	1/5	905.00

Source: own authorship (2026).

Table 2 shows, at the second and third columns, the calculated values of mean radius and polydispersion of atomic radii. The range of domain related to hardness goes from 130.20 to 1072 HV, while the range of δ covers 0.011 to 0.098.

Table 2

The mean radius of each HEA, polydispersion of atomic radii, and hardness.

HEA number	Mean radius (pm)	δ	Hardness (HV)
1	145.662	0.045	441.00
2	137.546	0.034	537.00
3	138.904	0.076	482.00
4	145.015	0.050	505.00
5	145.694	0.054	542.00
6	136.576	0.033	536.00
7	125.292	0.050	472.00
8	125.324	0.054	536.00
9	128.202	0.070	626.00
10	130.303	0.098	472.00
11	122.220	0.011	208.00
12	126.100	0.052	495.00
13	122.608	0.015	286.00
14	129.592	0.071	516.00
15	125.712	0.045	625.00
16	147.052	0.043	420.00
17	139.098	0.025	507.50
18	122.414	0.014	130.20
19	125.130	0.050	684.00
20	134.668	0.044	1072.00
21	122.608	0.015	286.00
22	122.996	0.014	296.00
23	125.324	0.040	263.00
24	134.830	0.090	800.00
25	125.518	0.054	484.00
26	126.294	0.050	407.00
27	132.405	0.095	590.00
28	134.183	0.090	740.00
29	123.675	0.026	636.00
30	128.234	0.056	905.00

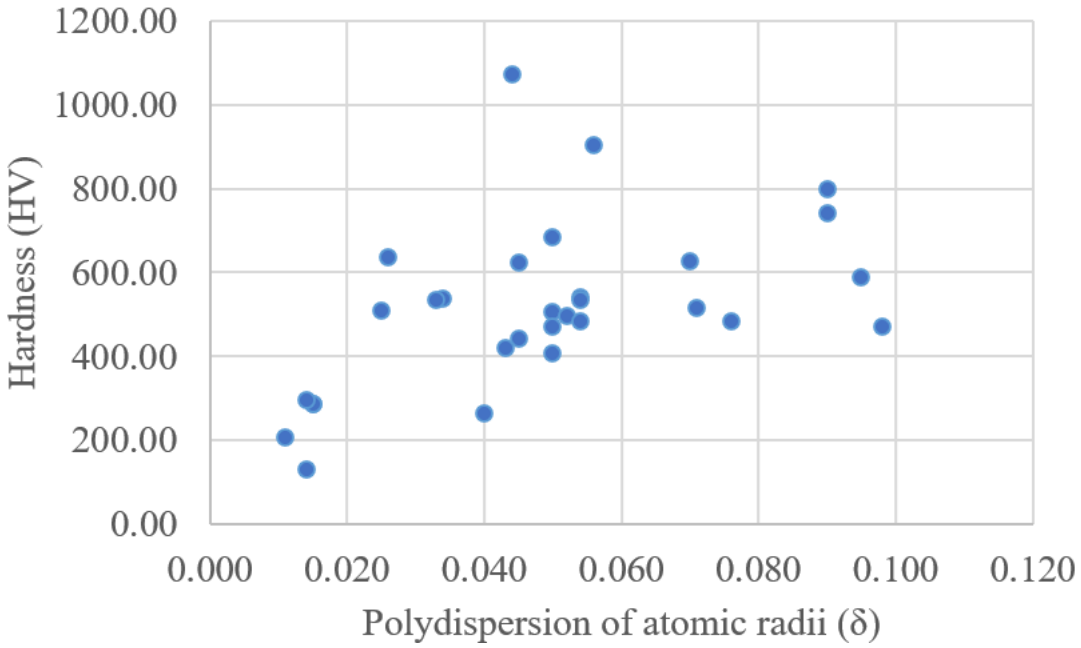
Source: own authorship (2026).

The thirty points corresponding to the listed HEAs are shown in blue circles in Figure 2. According to the dispersion of the points, the behavior of the curve does not allow the establishment of a unique function to map hardness related to polydispersion of atomic radii without a high magnitude of error. This is emphasized by the correlation factor of 0.50, which

is in the middle of low and high correlation. However, an attempt to predict the hardness of an alloy via the knowledge of δ is made here. Polynomials from first to 29th degree were tested, but they were badly conditioned. The polynomials with lower order degrees were built, however presenting a high level of error. In view of the impractical results presented, no equation is proposed to predict the hardness of these alloys.

Figure 2

Behavior of hardness of the thirty HEAs related to polydispersion of atomic radii.



Source: own authorship (2026).

5 FINAL CONSIDERATIONS

In this paper, thirty HEAs were the object of study aimed at investigating the relationship between Vickers' hardness and polydispersion of atomic radii (δ). The mean radius of the radii of the alloy elements was calculated to be input in the calculation of δ. Thenceforth, the correlation coefficient between Vickers' hardness and δ was calculated, and, finally, the relationship between both data was established.

In what refers to the thirty HEAs treated herein, the behavior presented between hardness and polydispersion of atomic radii yielded a relatively low correlation coefficient (0.50), which made establishing the relationship via polynomial equation difficult. Polynomials from first to 29th degree were tested, proving that either the error is too high or the polynomial is bad conditioned. Therefore, the main conclusion is that it is difficult to interpolate via polynomials due to the low correlation coefficient.

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