RELATIONSHIP BETWEEN ATOMIC RADII DIFFERENCE AND HARDNESS IN MULTICOMPONENT ALLOYS

RELAÇÃO ENTRE A DIFERENÇA DE RAIOS ATÔMICOS E A DUREZA EM LIGAS MULTICOMPONENTES

RELACIÓN ENTRE LA DIFERENCIA DE RADIOS ATÓMICOS Y LA DUREZA EN ALEACIONES MULTICOMPONENTES

10.56238/sevenVIIImulti2026-099

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ABSTRACT

Multicomponent alloys (MAs) are one of the most significant findings in what refers to metallic materials in this century. In this context, high-entropy alloys (HEAs) stand out by their wide range of possible combinations. The great number of possibilities requires robust prediction process to minimize the expenditure in experiments. In view of this, resources of research and development have been invested in the prediction of properties of MAs all over the world. Therefore, this paper investigates the influence of the atomic radii difference (Hume-Rothery's first law) on the hardness of thirty HEAs. Hardness values of these HEAs were extracted from literature in conjunction with the molar fraction of each alloy element. Thenceforth, the radius of each element was collected from the periodic table, and the atomic radii difference is calculated. The results of the relationship were expressed in terms of a plot involving both variables, and the coefficient of correlation. The low correlation coefficient and the behavior of the dispersion of the points in the plot of both variables showed that hardness does not depend on the atomic radii difference.

Keywords: Hardness. Prediction. Multicomponent Alloys. Atomic Radii Difference. Alloy.

RESUMO

As ligas multicomponentes (LMs) representam uma das descobertas mais significativas no campo dos materiais metálicos neste século. Nesse contexto, as ligas de alta entropia (LAEs) destacam-se pela ampla gama de combinações possíveis. A grande quantidade de possibilidades exige um processo de previsão robusto para minimizar os gastos com experimentos. Diante disso, recursos de pesquisa e desenvolvimento têm sido investidos na previsão das propriedades das LMs em todo o mundo. Portanto, este artigo investiga a influência da diferença entre os raios atômicos (primeira lei de Hume-Rothery) na dureza de trinta LAEs. Os valores de dureza dessas LAEs foram extraídos da literatura, juntamente com a fração molar de cada elemento da liga. Em seguida, o raio de cada elemento foi obtido

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da tabela periódica e a diferença entre os raios atômicos foi calculada. Os resultados da relação foram expressos em um gráfico envolvendo ambas as variáveis e o coeficiente de correlação. O baixo coeficiente de correlação e o comportamento da dispersão dos pontos no gráfico de ambas as variáveis mostraram que a dureza não depende da diferença entre os raios atômicos.

Palavras-chave: Dureza. Previsão. Ligas Multicomponentes. Diferença de Raios Atômicos. Liga.

RESUMEN

Las aleaciones multicomponentes (AM) son uno de los hallazgos más significativos en el campo de los materiales metálicos en este siglo. En este contexto, las aleaciones de alta entropía (AHE) destacan por su amplia gama de combinaciones posibles. Esta gran cantidad de posibilidades requiere un proceso de predicción robusto para minimizar la inversión en experimentos. Por ello, se han invertido recursos de investigación y desarrollo en la predicción de las propiedades de las AM en todo el mundo. Por lo tanto, este artículo investiga la influencia de la diferencia de radios atómicos (primera ley de Hume-Rothery) en la dureza de treinta AHE. Los valores de dureza de estas AHE se extrajeron de la literatura junto con la fracción molar de cada elemento de la aleación. Posteriormente, se obtuvo el radio de cada elemento de la tabla periódica y se calculó la diferencia de radios atómicos. Los resultados de la relación se expresaron mediante una gráfica que incluyó ambas variables y el coeficiente de correlación. El bajo coeficiente de correlación y el comportamiento de la dispersión de los puntos en la gráfica de ambas variables mostraron que la dureza no depende de la diferencia de radios atómicos.

Palabras clave: Dureza. Predicción. Aleaciones Multicomponentes. Diferencia de Radios Atómicos. Aleación.

1 INTRODUCTION

Technology is one of the main drivers in human progress. In what refers to materials, the branch of mechanical properties plays an important role because it dictates the effectiveness and efficiency of accomplishment of tasks. As progress takes place, the demand for improved or new materials turns out to be more evident (NONATO *et al*., 2025) (NONATO; RESTIVO, 2024b). The challenging demands stimulate the growth rate of improved or new concepts of materials. Nevertheless, many real-world problems do not have plausible solutions yet, which justifies the research and development in this area.

To obtain materials with mechanical properties within the required ranges, intense research is frequently demanded. This could be done in terms of experimentation, which often requires robust investment when dealing with significant uncertainty; and this could be done via computational predictions, which demands relatively lower capital expenditure, but may require reliable data. Anyway, the mechanical properties are planned, and the execution aims at reaching the planned range of properties (CALLISTER JUNIOR and RETHWISCH, 2020).

Mechanical properties are directly affected by the manufacturing sequence adopted, the elements selected to be part of the material, the quantity of the elements involved, among others (RESTIVO *et al*., 2023). Metallic materials, which are one of the main categories of materials, may consist of a unique element (pure metals), but may present two or more elements (metal alloys). In the case of metal alloys, one or more metals and/or non-metals are combined to obtain improved mechanical properties related to pure metals (RAZUAN *et al*., 2013). This may enable some applications to the alloys and/or improve the ranges of their mechanical properties. Those alloys with two main elements are called conventional, and those with three or main elements are the multicomponent alloys (SHUN *et al*., 2012).

Since conventional alloys are limited in terms of magnitudes of mechanical properties, this gap was partially fulfilled by the multicomponent alloys (MAs). However, a drawback about MAs is the available information due to infant stage in findings in this area, and due to the high number of possible combinations of elements (RESTIVO; RESTIVO, 2021). Therefore, MAs refer to metal alloys with three or more main elements and may include others in minor quantities. The configurational entropy distinguishes MAs in three categories: (a) low-entropy alloys (LEAs); (b) medium-entropy alloys (MEAs); and (c) high-entropy alloys (HEAs) (NONATO; RESTIVO, 2024a).

In the process of obtaining MAs, unplanned and undesired microstructures associated with insufficient magnitudes of mechanical properties may be obtained. To overcome this difficulty, predictive techniques have been increasingly used to minimize the necessity of

performing experiments to achieve the planned properties. Among the available techniques, calculation phase diagram (CALPHAD), thermophysical parameters calculation (TPC), machine learning (ML). One parameter (Hume-Rothery's first law) of TPC approach is studied (atomic radii difference) and related to hardness in this paper.

2 OBJECTIVE

The main objective is to observe and analyze the relationship between the atomic radii difference and hardness based on information related to hardness of thirty distinct equimolar HEAs, and the atomic radii difference, which is obtained via calculus.

3 METHODOLOGY

In this work, the methodology applies the 6-step workflow highlighted in Figure 1. Each step is described in the following paragraphs.

(a) First step: selection of data from literature: hardness values of 30 HEAs were collected from the reference (BORG *et al.*, 2020).

(b) Second step: Calculation of atomic radii difference (ΔR), in percent, which is made via the percentual relation between the difference of the largest, R_L, and the smallest radii, R_S, of the involved elements related to the radius of the smallest one (Equation 1):

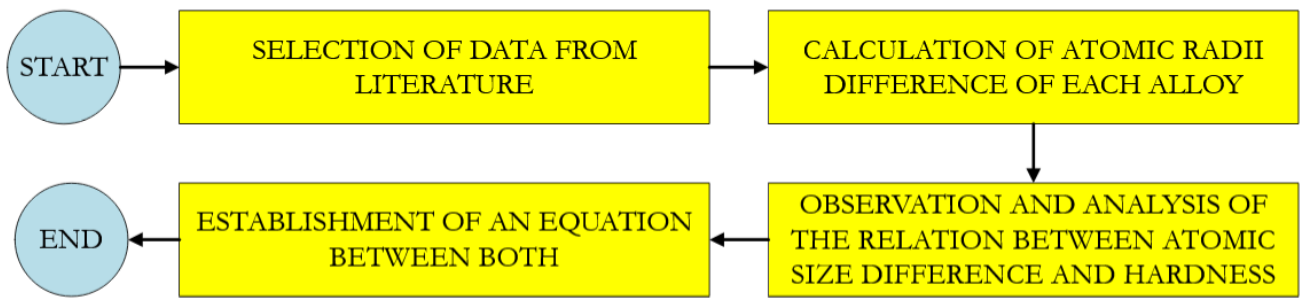
$$\Delta R(\%) = \frac{R_L - R_S}{R_S}\ 100. \qquad (1)$$

(c) Third step: observation and analysis of the relation between atomic size difference and hardness: study of the behavior of atomic size difference (in percent) and hardness (in Vickers).

(d) Fourth step: establishment of an equation between both parameters: proposition of an equation that helps in the prediction of hardness, given the composition of the MA.

Figure 1

Flowchart of the steps of this paper.



Source: Own authorship, 2026.

4 DEVELOPMENT

The methodology presented in the last section is executed in this section. The first column of Table 1 shows the high-entropy alloy code of each of the thirty HEAs as a code for further simplification in terms of nomenclature. The second column refers to the identification of the elements involved in the alloy composition and the molar fraction of each element. In this paper, the thirty HEAs are equimolar, and, therefore, the molar fraction of each alloy element is the unity divided by the number of elements in the alloy. The third column addresses hardnesses in Vickers, as presented in (BORG *et al.*, 2020).

Table 1

30 HEAs, with their code, composition, and hardness.

HEA code	HEA	Hardness (HV)
1	AlHfNbTaTiZr	441.0
2	AlMoNbTiV	537.0
3	CrNbTiVZr	482.0
4	HfMoNbTaTiZr	505.0
5	HfMoTaTiZr	542.0
6	MoNbTaVW	536.0
7	AlCoCrCuFeNi	472.0
8	AlCoCuFeNi	536.0
9	AlCoCuFeNiTi	626.0
10	AlCoCuFeNiZr	472.0
11	CoCuFeMnNi	208.0
12	AlCrCuFeNi	495.0
13	CoCrCuFeNi	286.0
14	AlCuFeNiTi	516.0
15	CoFeMoNiV	625.0
16	HfNbTaTiZr	420.0
17	MoNbTaTiW	507.5
18	CoCrFeMnNi	130.2
19	AlCoCrFeMnNi	684.0
20	CrMoNbTaVW	1072.0
21	CoCrCuFeNi	286.0
22	CrCuFeMnNi	296.0
23	CrCuFeMoNi	263.0
24	AlFeNiTiVZr	800.0
25	AlCoCrFeNi	484.0
26	AlCoCrCuFe	407.0
27	CuFeNiTiVZr	590.0
28	FeMoNiTiVZr	740.0
29	CoCrFeMnNiV	636.0
30	AlCrFeMoNi	905.0

Source: own authorship (2026).

In the first column, Table 2 presents the code of each HEA associated with the atomic radii difference (in percent) and hardness (in Vickers) in the second and third columns, respectively. The domain of hardness values goes from 130.200 to 1072.000 HV, while the range of $\Delta R(\%)$ covers 3.125 to 39.726%.

Table 2

The code of each HEA, its atomic radii difference, and its hardness.

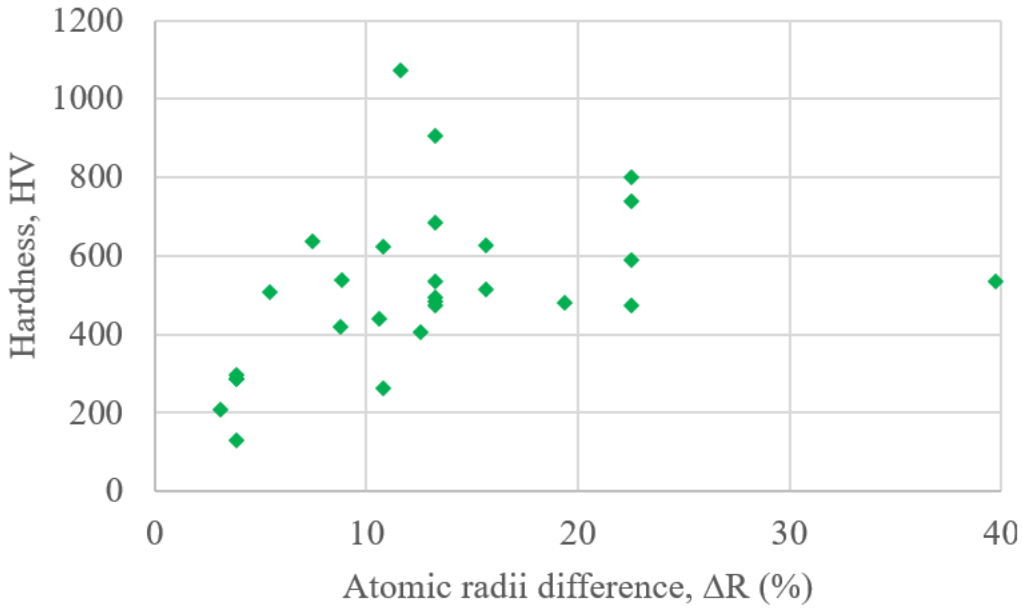
HEA code	$\Delta \boldsymbol{R}(\%)$	Hardness (HV)
1	10.625	441.000
2	8.844	537.000
3	19.375	482.000
4	13,125	505.000
5	13,125	542.000
6	39.726	536.000
7	13.287	472.000
8	13.287	536.000
9	15.646	626.000
10	22.500	472.000
11	3.125	208.000
12	13.287	495.000
13	3.876	286.000
14	15.646	516.000
15	10.791	625.000
16	8.750	420.000
17	5.442	507.500
18	3.876	130.200
19	13.287	684.000
20	11.644	1072.000
21	3.876	286.000
22	3.876	296.000
23	10.791	263.000
24	22.500	800.000
25	13.287	484.000
26	12.587	407.000
27	22.500	590.000
28	22.500	740.000
29	7.463	636.000
30	13.287	905.000

Source: own authorship (2026).

The plot of the 30 points addressing the HEAs listed in Table 1 are shown in green diamonds in Figure 2. The observation of the dispersion of the points by itself already denotes that the plot does not admit the formulation of a particular function to map hardness into the domain of atomic radii difference without a significant margin of error. This is emphasized by the correlation factor of just 0.01, which is a very low correlation. In view of this, based on the data of these thirty alloys, it is possible to affirm that hardness does not depend on atomic radii difference.

Figure 2

Behavior of hardness of the thirty HEAs in the domain of atomic radii difference.



Source: own authorship (2026).

5 FINAL CONSIDERATIONS

This paper was based on an investigation of the behavior of the relationship between Vickers' hardness and atomic radii difference in the universe of 30 HEAs. The hardness values were collected from the available literature, while the atomic radii difference was calculated from the information about the atomic radii of the elements involved in the formulation of the alloy.

The study related to both variables demonstrated that they are not correlated to the point of obtaining an equation to predict the hardness as a function of the atomic radii difference. Therefore, in the prediction of hardness of these thirty alloys, the atomic radii difference is irrelevant.

Further investigation is needed in the direction of collecting hardness data of more HEAs and/or studying the relationship of hardness with the other parameters in the TPC approach.

ACKNOWLEDGEMENTS

The authors would acknowledge the event organizers for the opportunity to share this work. The authors also acknowledge the research councils CNPq (proj. 408406/2021-6), CatalisaICT Sebrae (proj. 29083*128) and FAPESP (proj. 2023/09818-8) for financial support.

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