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Determination of a methodology for formulating constituent models of high entropy alloys

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Abstract*:* A program, based on static and dynamic regime tests and correspondent numerical simulations, was conceived to be appliedfor high entropy alloys mechanical characterization. The objective was to establish a combined experimental & numerical methodology for dynamic characterization of high entropy materials in high strain rate processes. The results of static tests were used to draw the characteristic diagrams of the real material. Based on the results obtained in the compression test, a numerical simulation was performed and a material constitutive model was determined in quasi-static conditions by an iterative process. In the formulating process of constitutive equations for high entropy materials, the dynamic experimental results obtained on SHPB were interpreted using similar simulated numerical models. The methodology conceived in this paper is applicable in materials science for the determination of the constitutive models of new materials.

1. Introduction

In the development of new metallic alloys designed to be used in special applications where the expected strain rates are extremely high, as ballistic protection applications, besides preliminary investigations, like chemical compositions and processing techniques effects on alloys properties [1, 2], a mandatory step is the mechanical behavior determination of such materials when they are subjected to deformation in similar conditions to those that may appear in real situations. That means determination of constitutive models able to reproduce experimental stress/strain diagrams for the interval of likely strain rate values. Besidestheir intrinsic value, such constitutive laws are crucial in numerical simulation analysis of mechanics of bodies subjected to rapid and severe deformations.

The subject of materials dynamic mechanical behavior is well represented in the scientific literature of the last decades. A first topic is represented by the development of new lab installations and testing principles used to induce high strain rates in the samples tested. The most notable achievements belong to Taylor [3] who proposed classical Taylor test and Kolsky [4], for its Split Hopkinson Pressure Bar

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installation, figure 1, where the states of sample were calculated using the elastic strains of installation bars recorded in time.

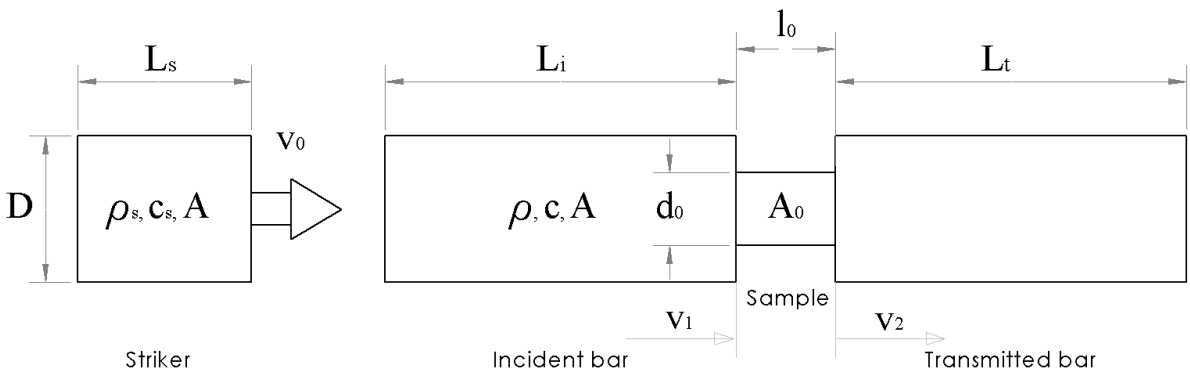


Figure 1. Schematic view of Split Hopkinson Pressure Bar.

Based on the fact that the sample enters during the test in adynamic equilibrium state, the engineering stress, engineering strain and engineering strain rate evolutions may be expressed as:

$$\sigma_e = E\frac{A}{A_p}\varepsilon_T \tag{1}$$

$$\dot{\varepsilon_e} = -2\frac{c_0}{l_0}\varepsilon_R \tag{2}$$

$$\varepsilon_e = -2\frac{c_0}{l_0}\int_0^t \varepsilon_R\, dt \tag{3}$$

where, in the equation (1), E is the elastic modulus of bars, A cross-section area of bars, A_p initial cross-section area of sample and ε_T transmitted elastic strain recorded in the bars. In equation (2) and equation (3) $c_0$is sound velocity of bars, l_0 initial length of sample and ε_R reflected elastic strain recorded in the bars. In the equation (4), equation (5) and equation (6), the true stress, true strain and true strain rate are given by:

$$\sigma = \sigma_e(1-\varepsilon_e) \tag{4}$$

$$\varepsilon = \frac{1}{1-\varepsilon_e}\dot{\varepsilon_e} \tag{5}$$

$$\varepsilon = -ln(1-\varepsilon_e) \tag{6}$$

A second topic is represented by the efforts of the scientific community to identify analytic expressions able to model the observed aspects as strain hardening, strain rate hardening and thermal softening [5] in materials mechanical behavior. This eventually led to proposal of several constitutive laws dedicated to high strain rates as Johnson-Cook model [6] or its simplified version where thermal softening is not accounted

$$\sigma_y = (A + B\varepsilon^{p^n})(1 + C\, ln\frac{\dot{\varepsilon}^p}{\dot{\varepsilon}_0}) \tag{7}$$

or Cowper Symonds model [7],

$$\sigma_y = (A + B\varepsilon^{p^n})\left[1 + \left(\frac{\dot{\varepsilon}^p}{\dot{\varepsilon}_0}\right)^{\frac{1}{q}}\right] \tag{8}$$

both, applicable to the metallic alloys that exhibit a viscoplastic flow. In the above mentioned laws, the influence of the viscosity on the plastic flow is isolated from the plastic strain hardening, each of thembeing a separate parenthesis. The identification of the coefficients of such parenthesis may be

done in different ways according to the available experimental data, i.e. in Taylor test the final dimension of the sample is used for a rough estimation of the mean stress and strain values, several such pairs being used to estimate the viscosity influence. Punctual values from the stress/stress diagrams were also used in the initial algorithm proposed by the Johnson-Cook for the strain hardening coefficient determination. More complex algorithms may use the computing power of the computers and the FEM software [8]. Such optimization algorithms [9] are designed to minimize the difference between the experimental data and computed ones, i.e. the final shape of the Taylor cylinder [10] or the stress/strain curves in SHPB tests [11]. Also, usually the plastic strain hardening coefficients are obtained from static tests data and strain rate hardening are obtained from dynamic tests data.

In the followings we will present a complete methodology used for mechanical characterization of a new metallic alloy that exploit the difference between the data obtained in FEM simulation of SHPB dynamic tests for a virtual case of no viscosity effect and the real experimental data to estimate the global influence of viscosity.

2. Test procedure and experimental data processing

The methodology contains four major steps:

1. Static tests and ordinary post-processing test data;
2. Correction of the static constitutive law by FEM simulation of the compression test;
3. SHPB dynamic tests;
4. Determination of the viscosity influence through FEM simulation of the SHPB compression test.

2.1. Static test data processing

If the tension test can be performed, the elastic modulus E of the material with high entropy is determined. However, if the manufactured specimendoes not allowsuch test, thenthe data obtained in the compression test will be used for such purpose. In compression samples, where an extensometer cannot be used, the displacement data is strongly influenced by the machine compliance. Modern universal testing machines are supple, having a minimal stiffness. Consequently, the measurement of displacement of the specimen' endincludes elastic deformation of the testing machine structure. Unwished effects of machine compliance must be eliminated. The correction procedure is based on the elasticity modulus E measured in a tension test and on the hypothesis of a linear elastic deformationoccurrence in the testing machine structure for the entire interval of attainable compression force values.

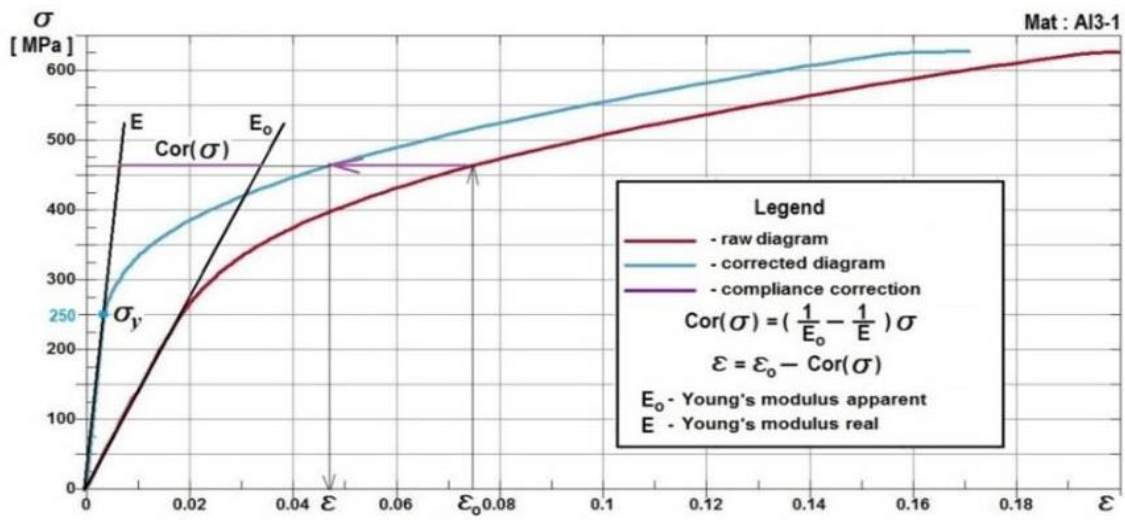


Figure 2. Compliance correction of engineering stress vs. strain diagram for Al3-1 alloy.

The raw test data of a compression test is a force/displacement table. Engineering stress vs. engineering strain curve may be deduced from such table, see figure 2. An apparent elastic modulus E_0characterizes the elastic portion of this curve. Removing the strain component given by the machine compliance using the formula from figure 2 will lead to corrected characteristic curve (blue curve in figure 3) where the elastic portion presents a modulus equal to E.Corrected data are still tabular. Figure 2 illustrates the procedure of compliance effect removal for Al3-1 HEA alloy.

Unlike the classical resistance calculations, where the deformations are very small, below the flow limit, to get accurate results in the plasticity with high deformations it is necessary to use the truestress vs. true strain diagrams, where the reference state is the current state, not the initial state as in the case of engineering diagram. The transition from the engineering diagram to the true one is done in two steps. The firstis to consider that the volume remains invariable (*a safe hypothesis when the plastic deformations areof an order of magnitude larger than the elastic ones*) and that there are no frictional forces on the specimen surfacesthat are in contact with the machine platforms. Given these conditions the deformed specimen would retain the cylindrical shape. In figure 3 the engineering - true transformation procedure for the Al3-1 alloy is synthesized.

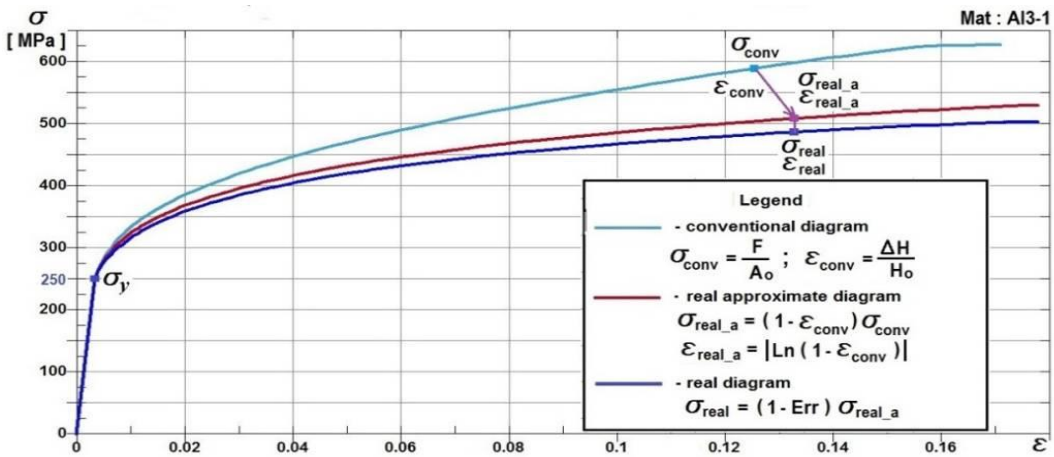


Figure 3. From engineering diagram to true diagram.

In the above assumptions, we obtain a first form of the true diagram (red curve) - still approximate - with the transformation relations presented in figure 3. In fact, the shape of the real deformed specimen, due to friction at the interfaces, does not remain cylindrical but gets a barrel shape.

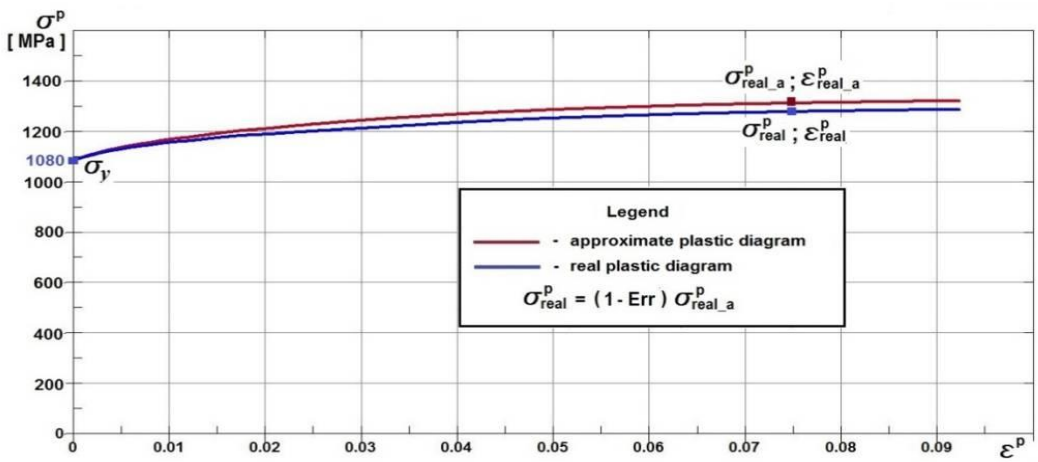
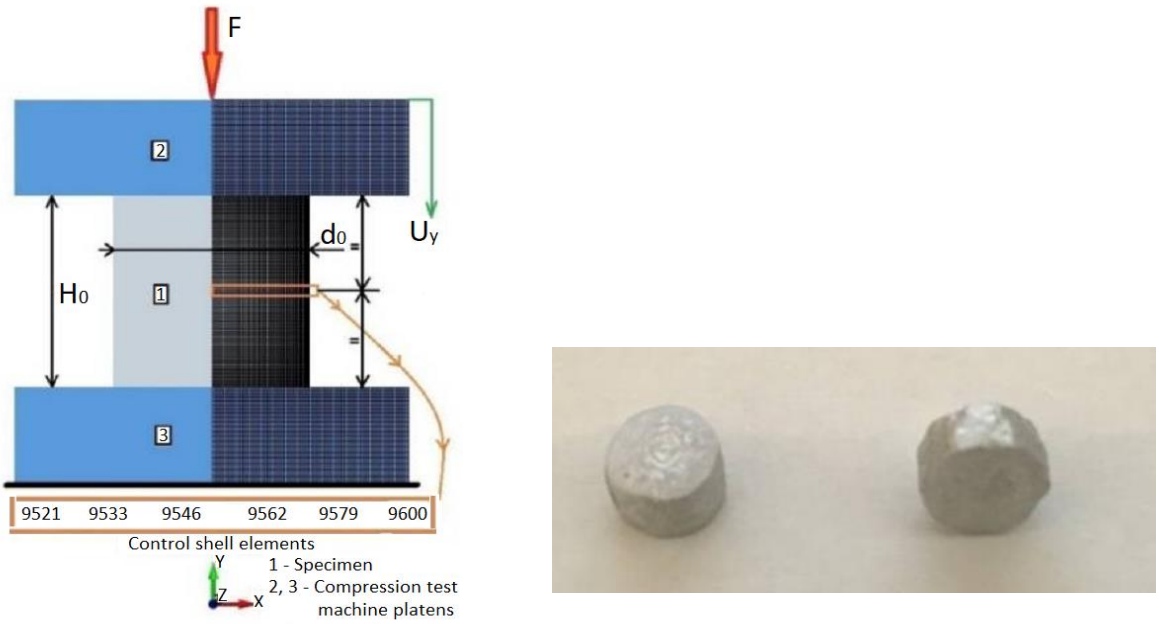


Figure 4. Plastic characteristic diagrams.

Eliminating the elastic component of the strain from the true characteristic diagram, we obtain the approximate plastic characteristic diagram of the tested material (figure 4).

In some applications where high precision is not required, experimental data processing can stop at this point. However, when more accuracy is needed the FEM is employed.

The specific configuration of a compression test on cylindrical specimens allows us to build an axially symmetric model such as that in figure 5. The axial symmetry gives the advantages of a small model and a fast solving.In the median plane of the specimen, 6 control elements were definedfor the true stresses and deformations monitoring. By controlling the relative displacement of the machine platforms, the specimen loading in the numerical simulation was identical to the experimental one. The surface friction at the specimen was taken into account. The approximate true stress/strain curve was used in the initially model for the specimen constitutive law. The FEM model was build and solved in LS-DYNA software [12].



(a) (b)

Figure 5. (a) 2D axial symmetric FEM model for compression test.
(b) Post test specimens shape.

The data get from simulation allow us to representthe compressive force as a displacement function. The simulated force $F_1$is given in figure 6. In the same figure the experimental recorded force F_0(after compliance compensation) is shown. The simulation error, E_{rr}, determined by the formula given in the top box of figure 6 is represented in the same figure. To simplify the calculation, the error has been linearized. The correction was then applied to the true characteristic diagram (figure 3) and to the plastic characteristic diagram (figure 4).The correction formulas can be found in the boxes on these two figures.

To confirm the solution, the numerical simulation of the compression test with the corrected material properties was repeated. The force-displacement obtained at the last simulation, the purple curve F in figure 6, overlaps F_0 with errors that tend to zero over the entire recorded curve F_0. After the last simulation, the used true stress/strain diagram was considered the constitutive law specific to mechanical behavior of material in the static regime.

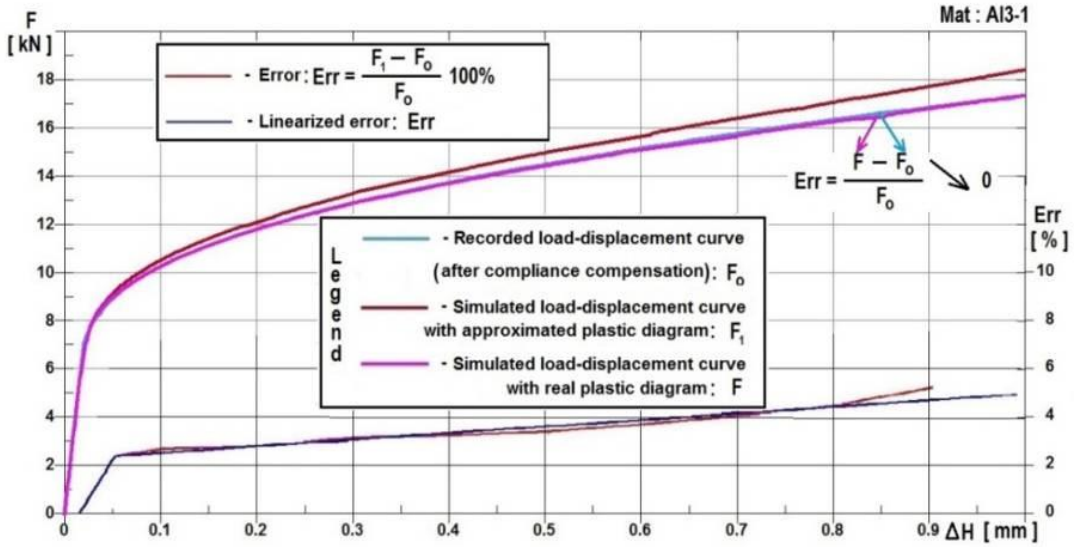


Figure 6. Force-displacement diagram.

2.2. Dynamic test data processing

The condensed expression of constitutive equations, like those of equation (7) and equation (8), dependent on the effective plastic strain and the plastic strain rate can be done with the relation:

$$\sigma_y = f(\varepsilon^p, \dot{\varepsilon}^p) \tag{9}$$

In practice equation (9)is usually formulated with separate variables in the form of:

$$\sigma_y = f_p(\varepsilon^p).f_v(\dot{\varepsilon}^p) \tag{10}$$

In equation (10) the function f_p represents the plasticity function, and f_v is the viscosity function. The plasticity function does not depend on the deformation speed and corresponds to the static tests. The plasticity function deduced for Al-3 alloy in the manner explained in the above subsection is plotted in figure 7, along with its binomial representation.

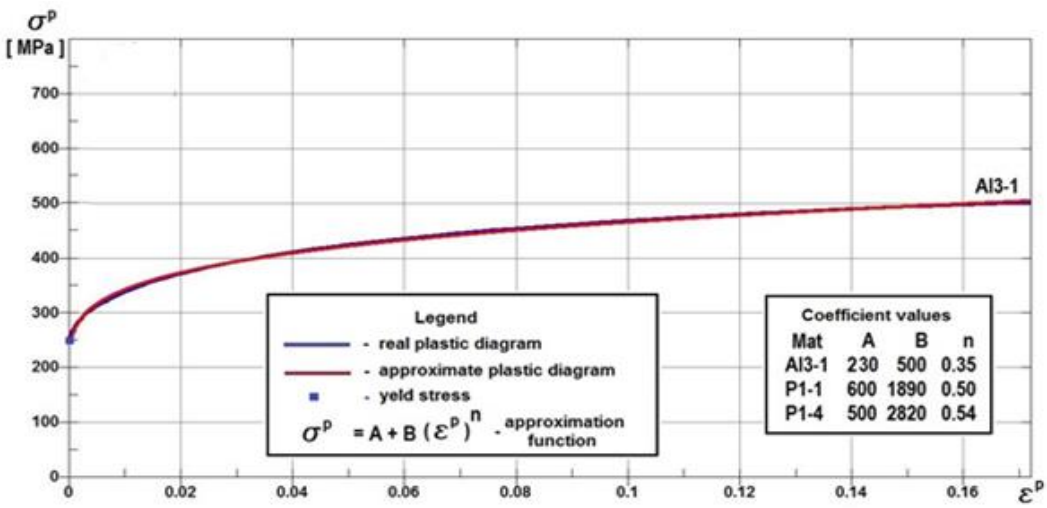


Figure7. Approximate and true plastic stress vs.plastic strain diagrams.

The viscosity function f_v can be determined through processing of specific data acquired during SHPB dynamic tests. From such dynamic test there is possible to obtain mean value for both strain and stress experienced by the tested specimen. During the planning of the tests, it was taken into account the fact that the viscosity function can be approximated sufficiently precisely with one parameter like in Johnson-Cook model. In this case a single pair of values $(\dot{\varepsilon}^p, f_v(\dot{\varepsilon}^p))$ is required for its estimation.

The method of determining the f_v function is based on a mediation procedure, combining experimental data with numerical simulations. Briefly, the viscosity function evaluation procedure, f_v, is described below, as follows:

- SHPB test (figure 1) on a cylindrical specimen and the acquired data processing (figure 8; figure 9);
- the determinationof the mean value for the specimen plastic strain rate during the experimental test $\dot{\varepsilon}^p{}_m$;
- the SHPB test is simulated in a 2D axial model and for the specimen constitutive law the expression determined in the quasi-static tests is used, without the viscosity function (figure 10);

$$\sigma_y = f_p(\varepsilon^p) \tag{11}$$

- the average value for the stress occurred in the specimen for both, the experimental and the simulation results, is determined and the viscosity function$f_v(\dot{\varepsilon}^p{}_m)$is determined by the ratio of the two average values (experimental and simulated) (figure 11);
- the determination of the viscosity coefficient of the constitutive law using the $(\dot{\varepsilon}^p{}_m, f_v(\dot{\varepsilon}^p{}_m))$ values pair;
- the SHPB test is simulated in a 2D axial model and for the specimen constitutive law a complete constitutive law is used, in order to evaluate the error.

The above procedure is exemplified for Al 3-1 alloy, based on the results of a test done with Ø20 mm SHPB from MTA on a 6 mm length cylindrical specimen of Ø6 mm with a projectile of 400 mm length at an impact velocity of 10 m/s.

In the figure 8 are shownthe elastic strains occurred into the SHPB during the Al 3-1 test. These curves are obtained from the electrical signals acquired during the test with the two Wheatstone bridges mounted on the bars of SHPB.

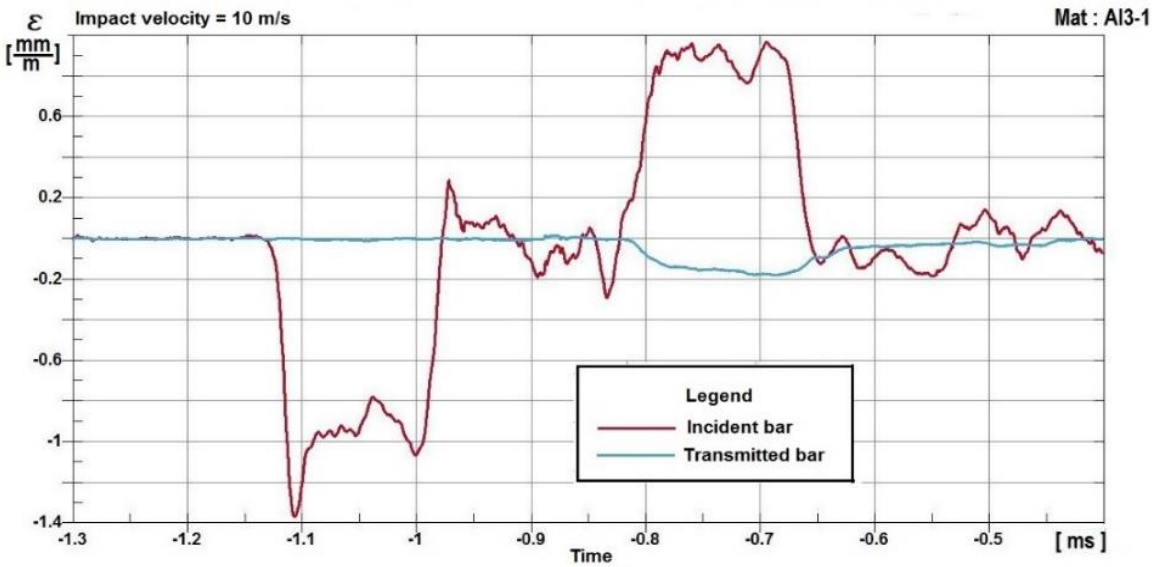


Figure 8. Elastic strains occurred in the SHPB bars.

The initial signal is then transformed in specimen engineering stress based on the equation (1) and reversed into the positive domain as in figure 9.

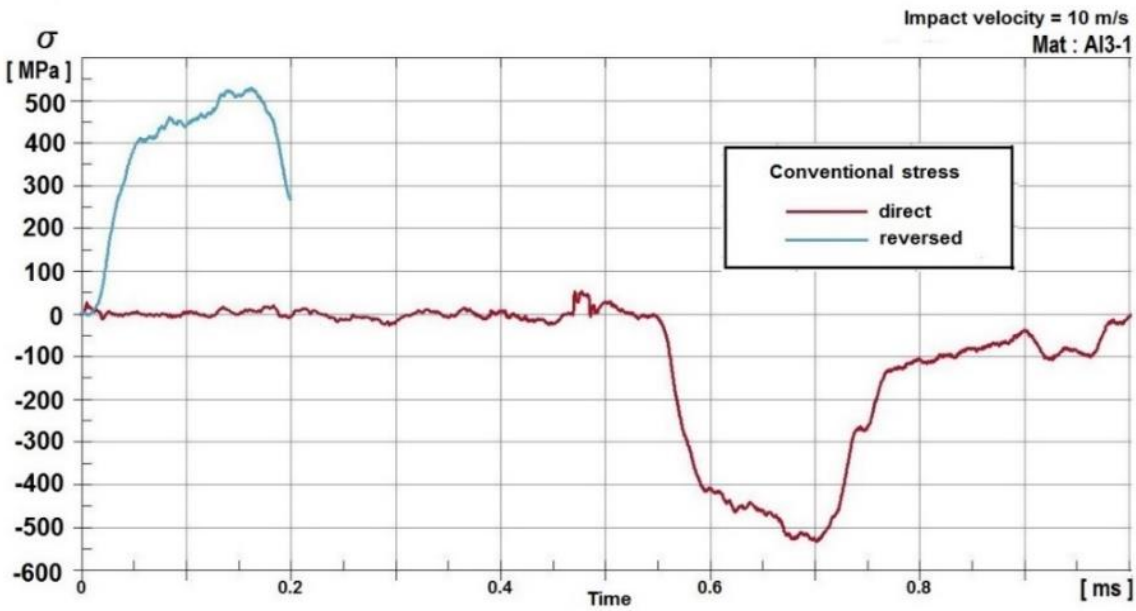


Figure 9. Processed specimen engineering stress.

From the SHPB numerical simulation for the specimen simplified constitutive law (without strain rate hardening component) given by equation (11), a similar engineering stress may be obtained using a gauge positioned on the center of the specimen, figure 10.

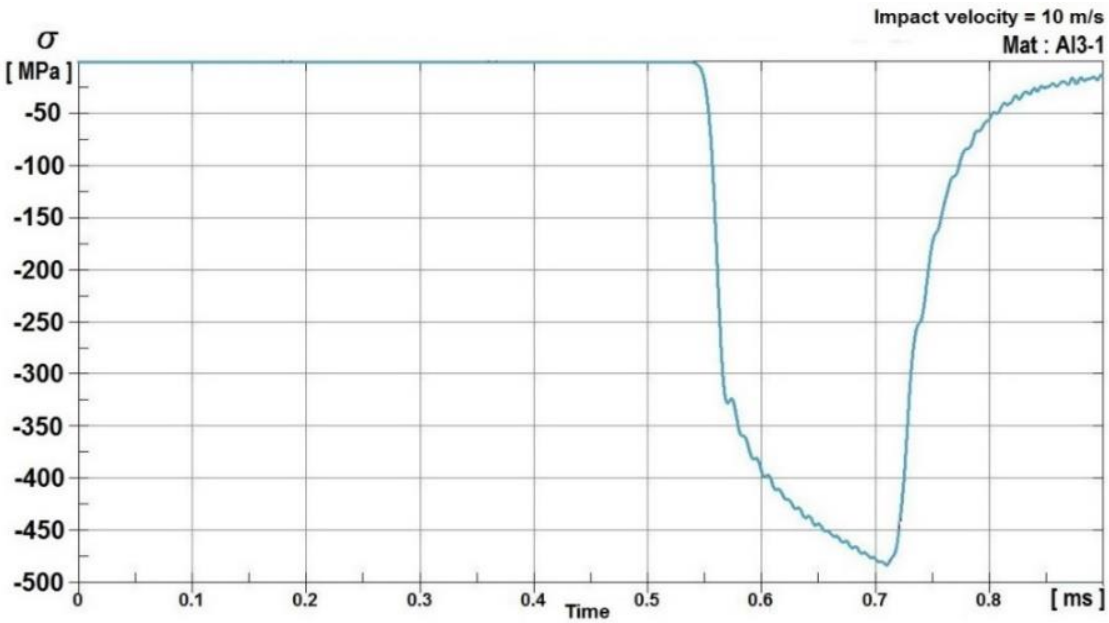


Figure 10. Specimen engineering stress evolution in time from SHPB numerical simulation.

The comparison of these two engineering stresses is shown in figure 11. The difference between these two curves is given by the viscosity manifested in the specimen during the real test. For each curve a mean value is calculated.

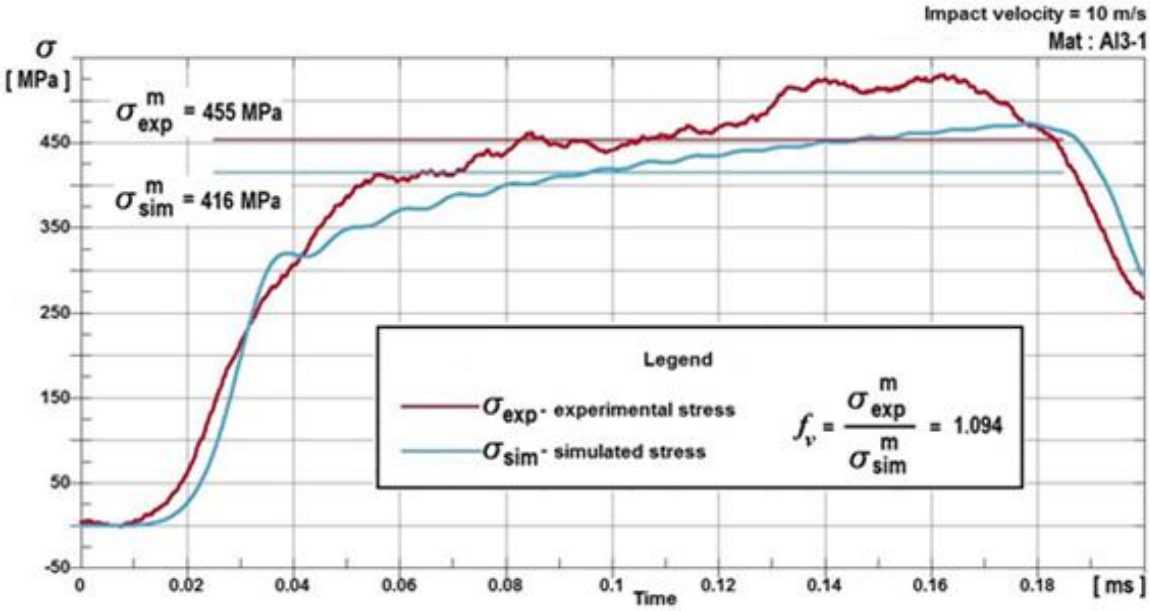


Figure 11. Engineering stresses comparison. Viscosity function.

The ratio of these two mean values is the value of the mean viscosity function f_v=1.094.This result combined with a mean value of strain rate,$\dot{\varepsilon}^p{}_m$ of 8000 s^{-1}and a reference value $\dot{\varepsilon}_0 = 1$s^{-1}allows the calculation of the strain rate hardening coefficient C from equation (7) as $C = 0.0104$.

3. Conclusions

Starting from the need to obtain a model for a class of high entropy alloys, we have developed a methodology that can be applied successfully for all new materials that exhibitviscoplastic flow.

The developed methodology is based on the reproduction of experiments using numerical simulation methods. Thus, the numerical simulation of the static tests leads to the determination of the plasticity function and the numerical simulation of dynamic tests performed with the SHPB are necessary to determine the viscosity function.

With the help of the numerical simulation implemented in the methodology, the errors in determination the real mechanical properties of the materials are eliminated.

The main disadvantage of this method is that in the dynamic area the average values of the engineering stresses are usedfor both, experimental and simulated cases.

The methodology is relatively compact, of medium complexity, a minimum number of tests being necessary.However, for a better accuracy of parameters determination a higher number of tests may be helpful.

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