Micromodeling of a dual-phase steel using an idealized micrograph generated by Voronoi diagrams

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Abstract. Dual phase (DP) steels are high strength steels used mainly in the production of vehicle bodywork, currently about 74% of the structural components are manufactured in this type of material. These DP steels are composed of a soft ferrite matrix with a hard, martensite phase. In this research, mechanical properties characteristic of these materials are linked, establishing dependence between volume fractions of each phase and simulations of the mechanical behavior in different situations are developed. Implementing a 2D bilinear plasticity model from the synergy of three design programs, regions of the martensitic phase of the material were generated in a 3D space. In the same way, these inclusions were parameterized and modeled together with a ferritic matrix. Then, using FEM to simulate 3D micromodeling (RVE), stress-strain diagrams are obtained. Finally, the results show deviations of 10% on average from the experimental values.

Keywords: Microstructure, tessellations, modeling, idealized micrographs, heat treatments.

1 Introduction

Dual phase (DP) steels are used in the production of vehicle bodies, currently about 74% of the structural components are made of this type of material, mainly due to the good combination of properties. DP steels are composed of a soft ferrite matrix and a hard phase, usually martensite. The mechanical properties of these steels depend on each phase (creep, hardness, etc.) and their volume fractions within the microstructure. In order to be able to establish the characteristics of each steel in particular, it is necessary to model their behavior to verify their response to different situations.

In researches that incorporate models of generation of granular structures with tessellations as a method to study particular conditions in steels, the development of an elastic-plastic finite element model of rolling contact fatigue of carburized steels, based on microindentation tests, stands out in order to determine influential factors in the generation of voids in the material such as grain size and orientation, the distribution of initial defects and inclusions of the material in the early growth of cracks, Aditya and Farshid [1].

The generation of a structure that simulates the experimental results by implementing quantitative and computational methods to achieve an ideal microstructure for Advanced High Strength Steel (AHSS) and High Strength Steel (HSS). These results are related in a variety of studies and researches where they analyze different configurations of the phases present in given samples, Shaeffler, Coates and Kimchi [2]. With the implementation of a software that allows to generate and define phases in microgranular structures in 2D and 3D in an interface which uses tessellations or Voronoi diagrams to build such structures. In this section, it is possible to understand in detail one of the main concepts present in the modeling of microgeometries, such as the cubic unit of measurement in three-dimensional objects called voxel; and how, in each of these models it is possible to distribute in an arbitrary way an arbitrary amount of dots generally called seeds which will later represent the grains of a microstructure, Martín, Tellaeche and Gil-Sevillano [3].

Although this type of research is limited to the construction of microstructures and its results are quite subjective as they do not incorporate quantitative properties present in each volumetric fraction, their existence defines a process aimed at linking experimental methods to improve the design of different metallic components.

Currently, research trends show an exponential increase in the modeling or simulation of components, in order to minimize prototyping and manufacturing costs, as well as to design the structure of a material to determine by means of simulations, complete or partial interpretations of the development and behavior of a steel, Giraldo [4]. And it is for this reason that this research is directed towards the optimization of microstructures presenting as a methodology the incorporation of software that allows to establish characteristics present in a dual phase steel and to generate volume fractions related to a bilinear plasticity model to define through a study based on metallographic tests the characteristics, conditions and mechanical response of this type of materials.

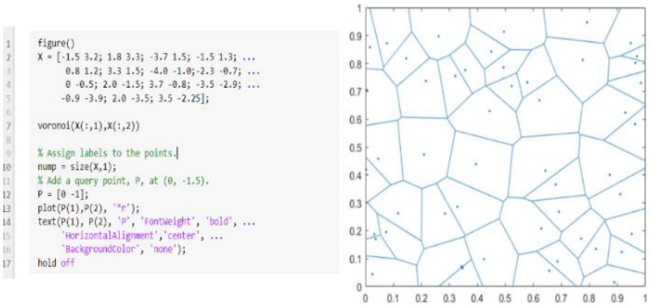
2 Methodology

The study was carried out based on the experimental results of research on the mechanical behavior of dual-phase steels obtained by heat treatments at intercritical temperatures. The importance of relating this research with theoretical-experimental data from previous practices allows measuring with greater precision the results expected from this type of studies.

The generation of granular structures was carried out by implementing the Voronoi diagrams method, which consists of constructing geometries based on random points in a Cartesian plane, these would then be converted into polyhedral regions determined by the disposition of each equidistant mediatrix to each point, Berg, Cheong and Kreveld [5]. This type of method allows not only to build granular structures, but is also used in tumor diagnosis, ship collision avoidance and GPS navigation, Lotero [6], Martinez [7]. In addition to the above, this technique stands out above Bebabbou's algorithm model, Katalin Bagi's constructive method and Laguerre's partitioning, as one of the most used in the modeling of microstructures due to the fact that it does not present limitations in the configuration of the size of the generated cells, Valera, Díaz and Casañas [8]. Thus, the grain size generated in each geometry constructed can be established as a parameter or determining factor of interpretation.

Using MATLAB®, a series of random Cartesian points were established in a 2D matrix that would initiate the creation of a polyhedral granular structure as shown in Figure 1, this would allow not only to determine the number of existing regions in the plane, but also to set the distance and section to be visualized in each geometric representation, MathWorks [9].

The experimental values of grain size expressed in microns and time spent in the furnace are shown in ascending order in Table 1. The 11 values corresponding to the last column of Table 1 were selected as the grain size range, which presents a minimum value of 28.3 μm and a maximum value 52.3 μm, with a standard deviation of 4.4 and a mean grain size of 41.92 μm, Vasquez [10].



```
figure()
X = [-1.5 3.2; 1.8 3.3; -3.7 1.5; -1.5 1.3; ...
      0.8 1.2; 3.3 1.5; -4.0 -1.0;-2.3 -0.7; ...
      0 -0.5; 2.0 -1.5; 3.7 -0.8; -3.5 -2.9; ...
     -0.9 -3.9; 2.0 -3.5; 3.5 -2.25];

voronoi(X(:,1),X(:,2))

% Assign labels to the points.
nump = size(X,1);
% Add a query point, P, at (0, -1.5).
P = [0 -1];
plot(P(1),P(2), '*r');
text(P(1), P(2), 'P', 'FontWeight', 'bold', ...
     'HorizontalAlignment','center', ...
     'BackgroundColor', 'none');
hold off
```

Figure 1. Representation of generated geometry in MATLAB

After obtaining the granular representations made in MATLAB® it was necessary to modify the format of each structure to perform a segmentation process of line elements as shown in Figure 2 and measure the grain size with the help of a computational design program, and thus determine whether the size of the cells generated is within the established range.

Table 1. Variation of grain size by time in oven at 770°C

	Time spent in [min]					
	0	**60**	**120**	**180**	**240**	**300**
Grain size in [µm]	12,3	13,78	20,78	21,64	23,84	28,3
	12,6	14,44	23,8	23,45	26,11	30,32
	13,2	14,86	24,32	26,6	31,8	35,09
	15,4	16,52	26,13	26,86	33,57	37,5
	15,7	17,15	27,78	27,43	35,78	39,52
	18,5	22,14	28,3	30,03	38,18	41,88
	20,1	22,38	28,71	30,44	38,54	44,02
	23,3	24,73	30,19	32,47	40,85	45,51
	24,1	25,7	33,39	35,93	43,82	47,31
	27,1	27,8	40,24	46,29	47,23	57

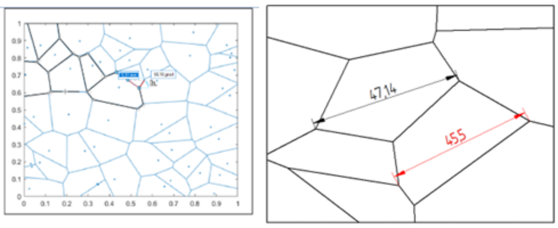


Figure 2. Construction by microstructure line segments and microstructure measurement with unit of measurement in µm

The structure is obtained with the appropriate format and region sizes or grain size determined by Table 1. The structure is exported to a finite element study program that allows identifying the properties of each phase and demonstrating its mechanical behavior under certain situations. In this first item, both the properties of each microconstituent and the percentage of volumetric phase present in each microstructure are related.

ZTaking into account the above considerations, the dual-phase steels, as their name indicates, are constituted by two phases called: Martensite, obtained by rapidly cooling the steels from their austenitic state at high temperatures (727°C) and is characterized by having a hardness of 50 to 68 RC with a tensile strength of 1667.13 to 2451.6 MPa, with an elongation of 0.5 to 2.5% and Ferrite, the softest constituent of the steel characterized by giving the material ductility, Castillo, Angarita and Rodríguez [11]. These constituents are always present with a phase percentage defined by the temperature at which the heat treatment is performed, so it is necessary to accurately determine the volumetric quantity of each phase. For this purpose, the values of each phase were taken as those present in the analysis of a micrograph as shown in Figure 3, this allows us to identify the amount of area for each constituent in the micrograph of the total area of the generated structure, Rodríguez and Álvarez [12]. After this, certain regions are selected in the structure called Voronoi 1 that would represent one of the aforementioned phases.

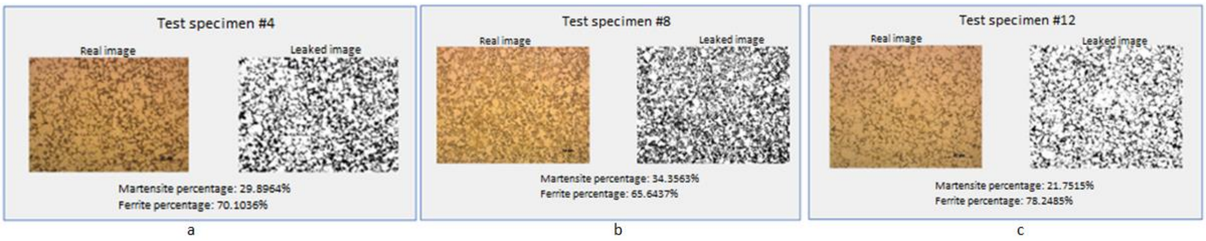


Figure 3. Filtered micrograph to determine the percentage of phases for a) Voronoi 1, b) Voronoi 2 and c) Voronoi 3

In this particular case, the Voronoi 1 structure presents a configuration of 29.9% martensitic phase (small islands with black color) at a ferrite interface of 70.1% (Figure 4). Once the process of microstructure construction and parameterization has been completed, it is necessary to establish these values in a data library within the program: Hardening coefficient of 0.001541 and creep limit 300 MPa for ferrite and 0.02875 and 1500 MPa for martensite respectively.

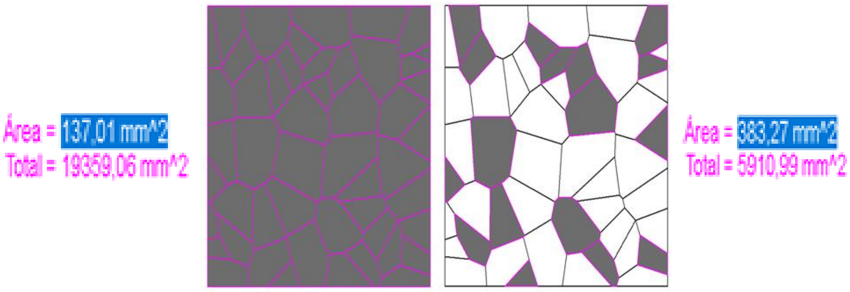


Figure 4. Filtered micrograph to determine the percentage of phases

Once the process of microstructure construction and parameterization has been completed, we propose the development of metallographic tests on three structures with different ares: Voronoi 1 with area of 0.0442 mm2, Voronoi 2 with area of 0.169 mm2 and Voronoi 3 with an area of 0.0156 mm2 each of these with phase percentages of 29.9% and 70.1%, 34.4% and 65.6%, 21.3% and 78.2% martensitic and ferritic phase respectively

The practice carried out was the modeling of micromechanical stresses based on micrographs, implementing as a model to follow an analysis by plasticity to the material, which aims to determine the mechanical properties with the maximum value quantified by studying the structure in conditions of plastic deformations, subjecting it to normal stresses that increase to overpass its elastic range and predict the capacity that can have each artificial structure generated to deform without breaking, Urbano [13]. As a first step to perform the practice on each structure, it is necessary to limit the horizontal and vertical movement by taking two sides of the idealized micrograph at 90 degrees with respect to each other, then restriction on the x-axis is applied for the vertical side, and in the opposite direction for the horizontal side, restriction or embedding on the y-axis.

For this particular study, there will be limitations on the left and lower lateral side. Since the practice is a study by plasticity, it is required to incorporate stresses as established by definition, and in this way increase these pressures until exceeding the creep limit of the material. For this research, line pressures are established on the right lateral side opposite to the movement restrictions already mentioned, and a general pressure is also incorporated, which will be evaluated as individual pressures since it is constituted by the selection of line segments at this end.

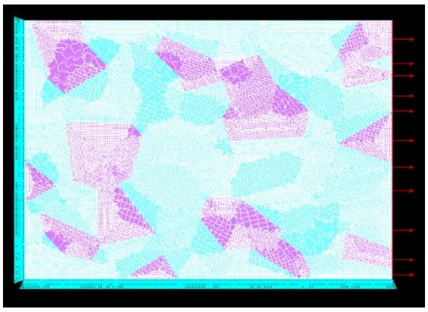


Figure 5. Line pressure and limiters on x and y axes

Subsequently, a mesh size was determined, which was established as a determining variable in the analysis of the results yielded by the system. It was established as minimum unit definition size in the structure the value of 10 and tailor-made as the study progressed, it was possible to demonstrate that the maximum definition size was 0.2. Then, the solution to the system is executed eliminating the condition of modification or local deformation in the structure, so that the deformations were presented inside the structure and not in its rectangular geometry. To finish this analysis with the representation of stresses and deformations present in the artificial microstructure, Figure 6.

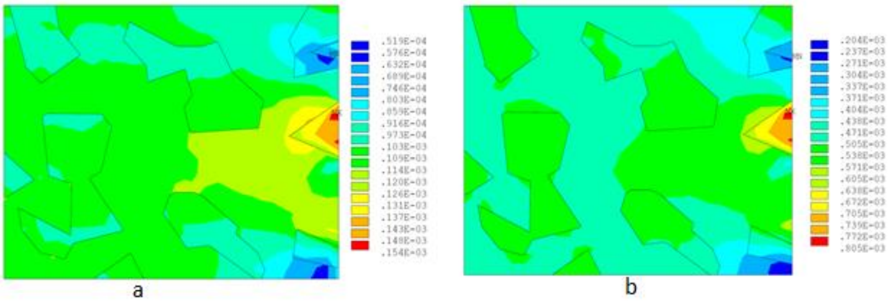


Figure 6. a) Stress values in Mpa for Voronoi 1, b) Deformation values for Voronoi 1

3 Results

The product of this research relates variables present in an artificial microstructure such as: region or grain size, volumetric fractions of microconstituents and pressures exerted in plasticity tests. Obtaining in this way 3 structures that behave as real micrographs, incorporating properties and characteristic values of these.

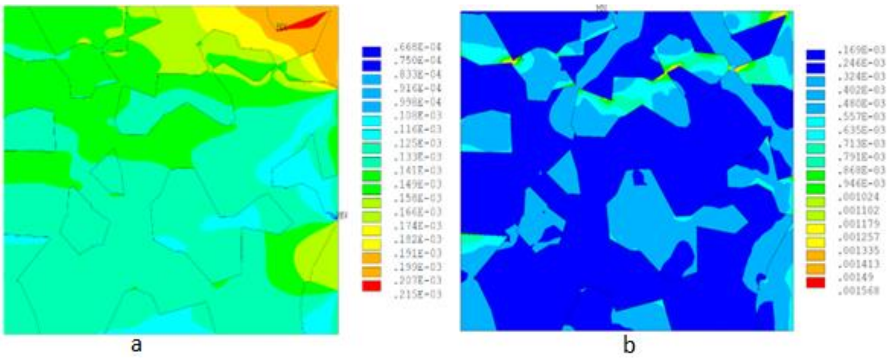


Figure 7. a) Stress values in Mpa for Voronoi 2, b) Deformation values for Voronoi 2

In Figure 7 we can appreciate the distribution of stresses and deformations in the structure called Voronoi 2 after performing the plasticity test in the system, in these illustrations it is evident the behavior experienced by the structure of 0.169 mm2 of area, with maximum stresses as the section approaches the vertical end where the pressures were located, likewise, the list on the right side of Figure 7 (a) shows the stress values and the regions where these are presented in a range where it is possible to state that the material retains its state of elasticity and no permanent deformations have been produced in the structure. Therefore, the distortion analysis performed had to interpret elastic and non-plastic deformations in the structure. Thus obtaining maximum deformations in 82% of the edges of material 1 established as martensite and material 2 as ferrite, which corresponds to possible points of generation of cracks or voids in the structure, these deformations would be studied as the research progresses.

Evaluating the results in the first tests, the study determined that in order to obtain a total performance in the tests performed on the microstructures, it was essential to perform a mesh refinement and determine characteristics, effects or patterns that could arise in each geometry and also to follow up on these, as the definition unit and the pressure exerted on the right vertical end varied. The values of maximum stress and strain were tabulated together with the number of nodes and mesh size, in order to determine yield times and variance of the data obtained.

Table 2. Maximum stress-strain values Voronoi 1

		At a pressure of 0.0008 Pa		**At a pressure of 0.002 Pa**	
Mesh size	**# Nodes**	**Stress values [MPa]**	**Percentage of deformation**	**Stress values [MPa]**	**Percentage of deformation**
9	1606	202	0,001085	1433	0,221631
5	4190	207	0,001079	1656	0,323304
3	10385	209	0,001075	1815	0,358838
1	83776	213	0,001071	2128	0,542068
0,5	325229	213	0,001071	2655	0,577122
0,2	476312	213	0,001059	3182	0,612176

Table 3. Maximum stress-strain values Voronoi 2

		At a pressure of 0.0008 Pa		**At a pressure of 0.002 Pa**	
Mesh size	**# Nodes**	**Stress values [MPa]**	**Percentage of deformation**	**Stress values [MPa]**	**Percentage of deformation**
9	660	154	0,000806	384	0,001911
5	1134	156	0,000811	398	0,002298
3	2713	155	0,000806	389	0,002703
1	21168	158	0,000823	449	0,003365
0,5	79991	160	0,000836	496	0,004579
0,2	486326	160	0,000852	528	0,004852

Table 3. Maximum stress-strain values Voronoi 3

		At a pressure of 0.0008 Pa		**At a pressure of 0.002 Pa**	
Mesh size	**# Nodes**	**Stress values [MPa]**	**Percentage of deformation**	**Stress values [MPa]**	**Percentage of deformation**
9	200	118	0,023334	4953	0,425037
5	360	149	0,027826	7422	0,503019
3	850	153	0,030063	8434	0,545916
1	6785	168	0,043742	11885	0,698813
0,5	26070	170	0,054861	15579	0,810616
0,2	35014	170	0,065980	17410	0,922419

4 Discussion and conclusions

The research concludes with the modeling of three artificial microstructures by implementing the Voronoi geometric construction method to recreate the microstructure present in a micrograph of a dual-phase steel. With the realization of this study, analysis conditions were determined such as volume fractions and parameterization of microconstituents, failure mechanisms formed in the plasticity practice carried out to each structure and how they behave when evaluating their stress and strain values graphically.

One of the key moments addressed by this project was to identify what percentage of phases should be used to perform the modeling of each structure, in the first place, what was sought was to adopt the exact geometry of a micrograph of a dual-phase steel. When performing the first mapping tests in the computational design program, the structure generated to scale showed great symmetry with respect to the selected micrograph, but when exporting this structure generated by this process to the finite element program to perform the test simulations, errors occurred in the selection of areas or grains. This is due to limitations in the sketching process: when selecting a visual representation (image) it must have a fairly high resolution so that the system can accurately identify each line segment to be constructed. In this particular case, the constructed geometry was elaborated with non-existent line segments or connector nodes in the center of some regions, these conditions would prevent the execution of this method.

Based on the above, the alternative proposal was to determine the percentage of each constituent and geometry of the microstructure by implementing the image filtering tool in the MATLAB® program, which is capable of quantifying the amount of area per component that could be present in each micrograph Figure 3 b and c, then select the regions that would constitute a volumetric portion of each component and identify within these the characteristic properties of these in the artificial microstructures.

By plotting the data obtained for the Voronoi 3 structure in Table 3, Figure 8, it was possible to visually determine the behavior of this structure in a stress-strain diagram and to identify the percentage of deviation of the experimental values obtained from the plasticity test and compare them with the theoretical values in the practical stress test performed on specimens in the mechanics laboratory.

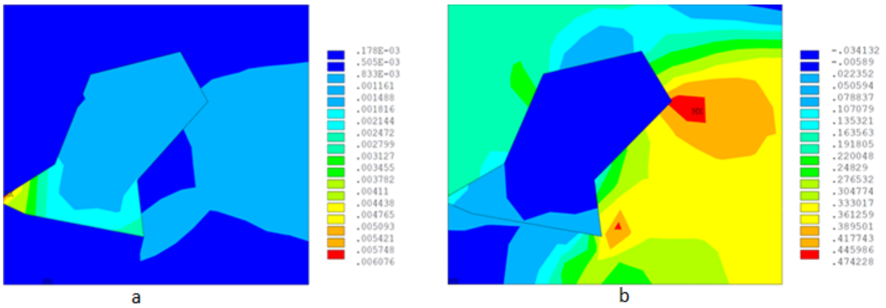


Figure 8. a) Stress values for Voronoi 3, b) Deformation values for Voronoi 3

In this way, an engineering stress vs. strain diagram is obtained for specimens 7, 8 and 9 in parallel with the real stress vs. strain diagram for microstructure 3 with characteristics of an isotropic bilinear material: with a first increasing straight line representative of the elastic zone of the material with small deformations as its stress values increase, and followed by a curve with deformations that increase exponentially in a reduced stress range, thus representing the zone of plastic or permanent deformations in the material. Establishing as a percentage of deviation between the stress values in each practice of 2.5% and deformation with average dispersion values that do not exceed 11.3%, concluding that the microstructures generated have great affinity with respect to the behavior experienced by this type of steels exposed to axial tension practice.

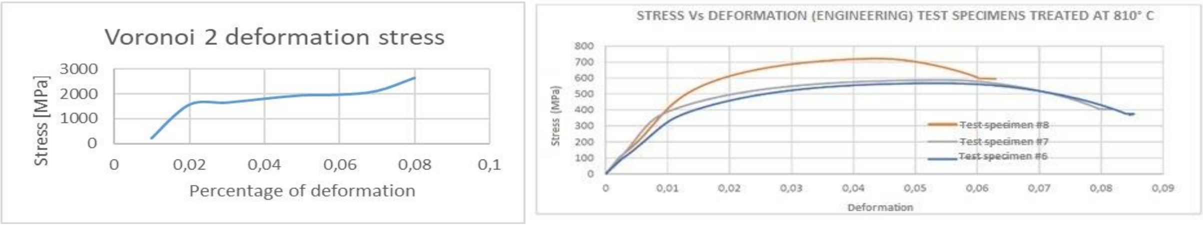


Figure 9. Stress vs. strain diagrams for artificial models and comparison of results

On the other hand, the study affirms that the generation of failure mechanisms mentioned in the introductory section of this research, with the generation of voids in the interface of the materials are presented in the artificial microstructures, taking into account that 82% of the resulting representations of the deformation analysis in structures, denoted maximum distortions in the common edges of the components Figures 7 (b) and 8 (a). Thus, indicating how the modeling of this type of structures based on the generation of geometries by the Voronoi method and the synergy between different computational programs aims to mechanically recreate the behavior in situations of a material or component.

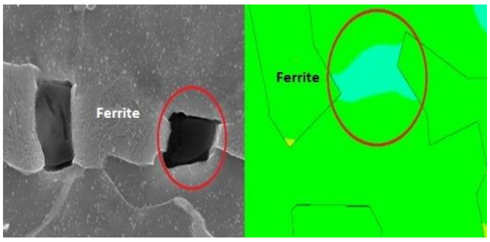


Figure 10. Comparison of micrograph behavior and idealized microstructure generated by Voronoi diagrams

Some factors that can be means of study in future research are: the variation in the dimensioning of the generated structures, in principle the project was aimed at making structures with different areas, but taking each artificial geometry created with a measure of 10 mm thick as a constant in the research. Therefore, we can affirm that the modification in the dimensioning was carried out in a partial way and we could produce different results when elaborating a total modification to the structures.

On the other hand, the results obtained from the plasticity test were performed under a bilinear analysis, with which visual representations of the mechanical behavior of each structure were obtained, stress vs. deformation diagrams and failure mechanisms such as the generation of voids in the material, data and effects that can be compared when performing this same study under a multilinear analysis and determine how similar is the behavior of these structures in both tests or how much they vary from each other. As well as the production of three-dimensional structures and the study of these structures.

Acknowledgments. To the Universidad Distrital Francisco José de Caldas and the computational mechanics research group GrupLAC that allowed the use of their data to carry out this research.

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