

Mathematical Modeling of Phase Transformations and Residual Stress in A Thermomechanical Heat Treatment in AISI 1045 Steel

By FEM

Karen Magally Valenzuela Romero¹, Carlos Arturo Bohórquez Ávila²

¹Department of Mechanical engineering, Libre University, COLOMBIA
Email: karenm.valenzuelar@unilibrebog.edu.co

²Department of Mechanical engineering, Libre University, COLOMBIA
Email: carlosa.bohorqueza@unilibrebog.edu.co

Abstract— Materials with high mechanical characteristics are ideal for many applications primarily in the automotive industry like the TRIP (Transformation Induced Plasticity) steel, but its high cost to determine their properties limit their study, for this reason the mathematical and computational modeling have emerged as a possibility of analysis and study of the properties of the material. One of these techniques is the micromodeling mathematical analysis using a representative elementary volume (RVE), used for the determination of residual stresses through programmed into the APDL of ANSYS ® software. Previous research has taken commercial DP steels (Dual Phase) or steels with high percentage of alloying elements, there is no evidence of studies in medium carbon steels treated from intercritical temperatures. The finite element method (FEM) has been a tool used in predicting the behavior of steel for his accuracy in the results. In this research the mathematical modeling that was done to a thermomechanical treatment in AISI 1045 steel, through the MEF is displayed. As initial results experimental data were taken to evaluate the convergence of the results. In determining percentages of microstructures we use JMARK equations, which were implemented in the MATLAB software. The elastic and plastic properties were taken from references to be used in a plastic bilinear model analysis. The effects of the simulations show the percentages of microstructures that were to be found after the thermomechanical treatment. The results of this study show the accuracy between the experimental and the simulated results.

Keywords— Mathematical Modeling, AISI 1045 steel, thermomechanical treatment, FEM, residual stress

I. INTRODUCTION

Currently the high-strength steels are imposed as potential candidates for applications where you want to optimize the elation stress-weight and that need to be manufactured in metallic materials, one of the industries interested in this type of steel is the automotive because a reduction in weight means fuel savings. [1]

Steels have different capacities of tensile strength and strain as can be shown in Figure 1, there are high formability as are the interstitial steels (IF) with red color at left side , these have low tensile , so conversely are martensitic steels (MART) with light blue color at right side which have a low percentage of deformation but high tensile strength , from this requirement a new generation of steel which has both properties in a balanced manner as it is arises steel TRIP (Transformation Induced Plasticity) with green color in the center.

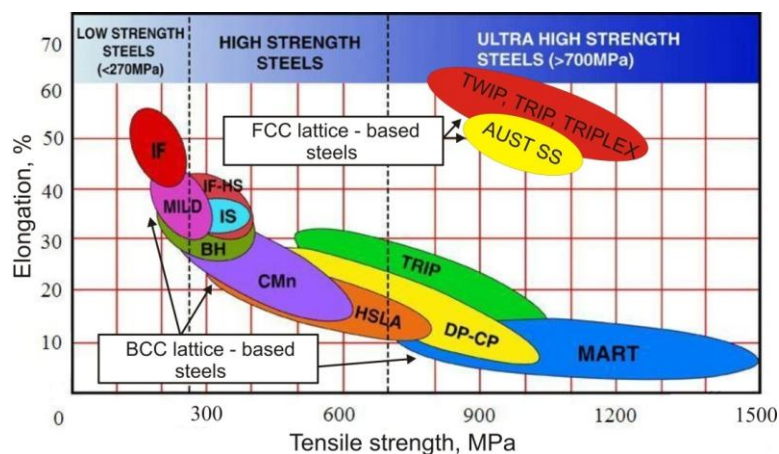


FIGURE 1. STEEL CLASSIFICATION

Which are characterized by the balance between strength and ductility , this is due to the microstructure formed of ferritic matrix , which is observed in Figure 2 , this provides desired ductility , a volume fraction of bainite and retained austenite in

low percentage , giving the steel special properties such as ; good deformation , high fatigue resistance , high impact energy absorption and a high elastic limit , thanks to these properties the induntrie can be made complex parts for automobiles but at the same time safely . [2]

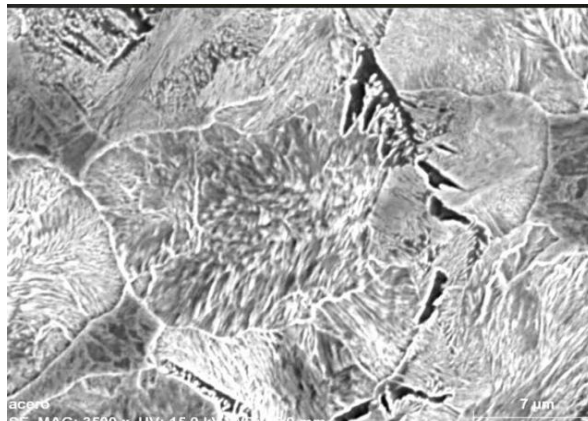


FIGURE 2. MICROSTRUCTURE OF A TRIP STEEL

The development of experimental research in these steels is limited due to high costs for that reason will make use of mathematical modeling finite element (MEF), according to ASM 2020 most research in the field of treatments thermal and thermomechanical who wish to make first must go through a mathematical modeling to assess its feasibility avoiding unnecessary costs. [3-4]

Moreover, it is necessary to consider the thermomechanical treatments which combined plastic deformation with thermal treatments in order to produce microstructures and improvements in the mechanical properties of the material, which would not be achieved if conducted independently. [5] The primary objective of this treatment is to improve the mechanical strength without reducing the ductility of the steel treated. The first part of this treatment is to perform a plastic deformation which will cause the material undergoes a transformation phase which may be diffusive or diffusive, due of this appear the most important microstructure called bainita in TRIP steels. The interaction of the variables involved in a heat treatment is illustrated in Fig. 3, where you can see the speed with which change the temperature influences the phase transformations that occur, and these in turn to occur generate latent heat, on the other hand changes in the temperature rise to thermal stresses, such that in turn influence the phase transformations and deformations caused in the treated parts. [6-7-8-9]

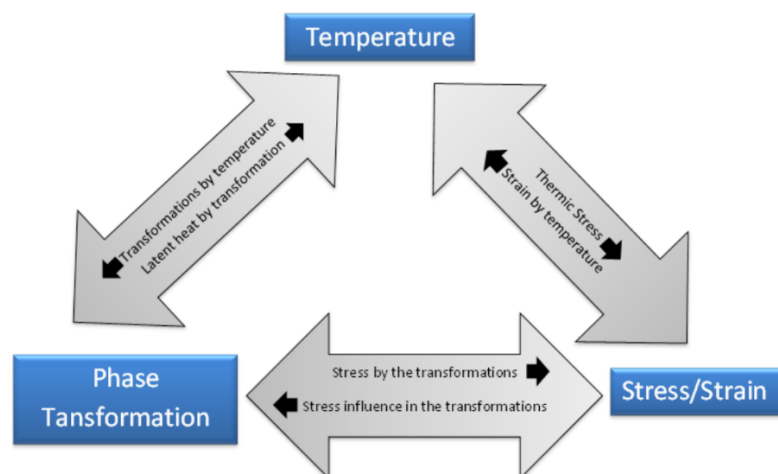


FIGURE 3. SCHEMATIC REPRESENTATION OF THE INTERACTION OF TEMPERATURE FIELDS, AND PHASE TRANSFORMATION EFFORTS

Is used as a reference, the chemical composition of AISI 1045 steel , this is used commercially by the average percentage of carbon steel is additionally a low cost since whose properties ; strength, toughness , good surface finish , machinability , can also support stress up to 600 MPa , for these conditions is ideal for applications in the automotive and agro- industry. [5]

II. MATERIALS AND METHODS

For the realization of this project was necessary to take the study (J. Quezada,) entitled "Estudio microestructural de un acero 1045 tratado termomecánicamente". In which 1045 steel specimens were taken , measuring 1 inch long and ½ inch in diameter, has the chemical composition of steel in Table 1. [10]

TABLE 1
CHEMICAL COMPOSITION OF STEEL 1045 .

C%	Si%	Mn%	P%	S%	Cr%	Ni%	Mo%	Sn%	Cu%	Al%
0.46	0.21	0.009	0.009	0.017	0.024	0.029	0.003	0.004	0.045	0.001

Subsequently compressing the specimen is performed, in which loads of 15, 20 and 25 tons, for each one of these 5 specimens loads the deformations are shown. [10]

TABLE 2
PERCENTAGE OF AVERAGE STRAIN ACCORDING TO THE LOAD

Load (Ton)	% Average strain
15	9.28%
20	23.6%
25	36.14%

After deformation the heat treatment is performed by the next sequence show in Fig. 4. [10]

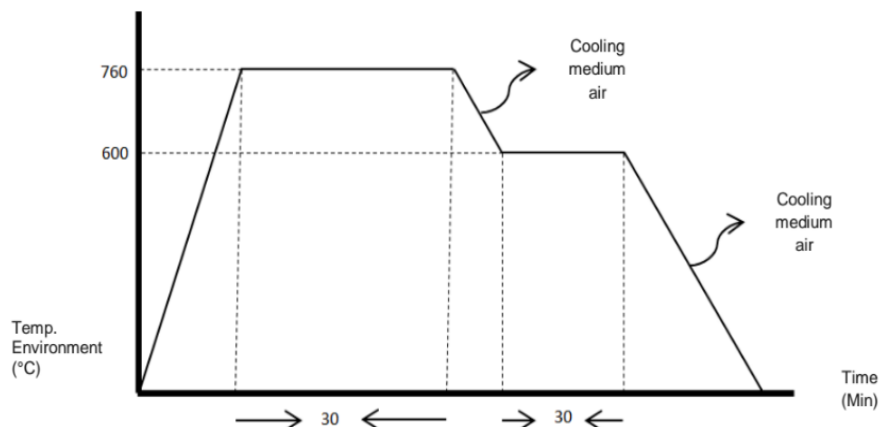


FIGURE 4. SEQUENCE OF HEAT TREATMENT FOR STEEL 1045

At the end of the process with each specimens its obtained the metallographic, that then is used in this study.

This project was development in two parts; the first part consisted in model the temperatures and percentages of microstructures that develop in a thermomechanical treatment using a constitutive model in which different deformations are taken, like; temperature, TRIP, phase transformations, plastic and elastic deformation, resulting in the following equation: [1]

$$\varepsilon = \varepsilon^{Tem} + \varepsilon^{Trans} + \varepsilon^{Plas} + \varepsilon^{TRIP} \quad (1)$$

In order to model mathematically temperatures and phase transformations JMARK equations are taken. [11-12-13]

$$\frac{dv}{dt} = K(T)^{1/n} * n * (1-v) * (\ln 1/1-v)^{(n-1)/v} = f(T) * g(V) \quad (2)$$

Where,

V = Volume fraction of the phase

T = Temperature at which you want to know the volume fraction of phase

t = Time

k and n = Constants related to processing of the experimental data obtained

f (T) = Temperature function

$$f(T) = A * (T_{Trans} - T)^n * \exp(-Q/RT) \quad (3)$$

g (V) = Volume fraction function

$$g(V) = \frac{V^{0.4(1-V)} * (1-V)^{0.4*V}}{a - b * V} \quad (4)$$

Where in the two previous equations,

A, a, b and n are constants showed at Table 3.

Q = Activation energy

T_{Trans} = Transformation Temperature

R = Gas constant, 8,314J / (mol * K)

V = Is the volume fraction of transformed microstructure.

TABLE 3
CONSTANTS FOR FUNCTIONS f (t) and g (v).

Structure	$A(1/s - K^n)$	n	Q(kJ/mol)	$T_{Trans}(^{\circ}C)$	a	b
Ferrite	0.213	3	115.546	766	0.75	1.2
Perlite	2.38	3	115.546	719	1.41	0.37
Bainite	213	2	115.546	651	0.44	0.32

$$\frac{dV_m}{dt} = 0.0428(M_s - T)^{0.191} * V_m^{0.382} * (1 - V_m)^{2.421} \quad (5)$$

Where,

V_m = Volume fraction of martensite.

M_s = Martensitic transformation temperature, given by equation.

$$M_s = 512 - 453C - 16.9Ni - 15Cr - 9.5Mo + 217C^2 - 71.5CMo - 67.6C * Cr \quad (6)$$

The purpose of these equations is to build a diagram TTT (Temperature, Time, Transformation) in the MATLAB® software and determine the time what the microstructure to be found.

In order to determine the residual stress of the material is made use of programmed in the APDL ANSYS ® software, we take the metallographics with an extension to 500x, the metallography was divide in small squares in SolidWorks software, where in the opinion of the authors of project was determined in each square which was this material if ferrite (yellow color) or ferrite (black color). Each of this microstructure has unique properties which are required to have for simulation in ANSYS ®, these are shown in table 4. [14-15-16]

TABLE 4
MECHANICAL PROPERTIES OF PERLITE AND FERRITE MICROSTRUCTURE

Property	Ferrite	Perlite
Young modules	211.9 Gpa	210.3 Gpa
Poisson Coeficient	0.2888	0.2877
Yield stress	500Mpa	710Mpa
Tangent module	1541 Mpa	1680.8 Mpa

To show the steps taken for simulation in ANSYS ®, see the Fig. 5:

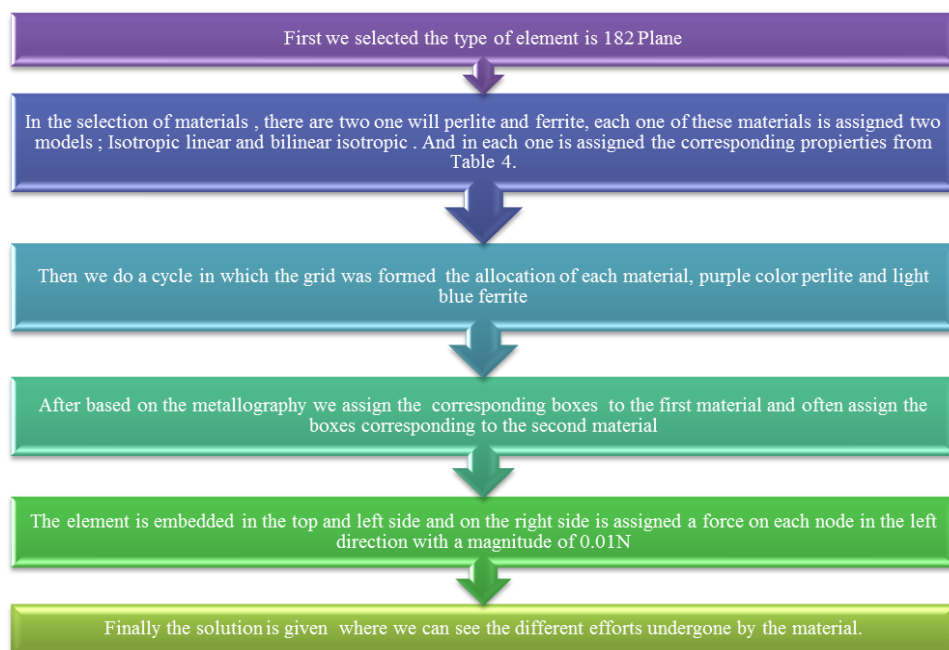


FIGURE 5. STEPS FOR SIMULATE ADPL IN ANSYS® software

III. RESULTS

From equations JMARK which were implemented in the Matlab software throw results in Fig. 5. In which can be seen as varying the time and temperature different microstructure of 1045 steel are obtained with respect to composition chemistry study was obtained from the experimental part. The cooling rate is low because it should take air velocity to prevent the formation of martensite and to obtain a malleable steel and TRIP steel resistant characteristic

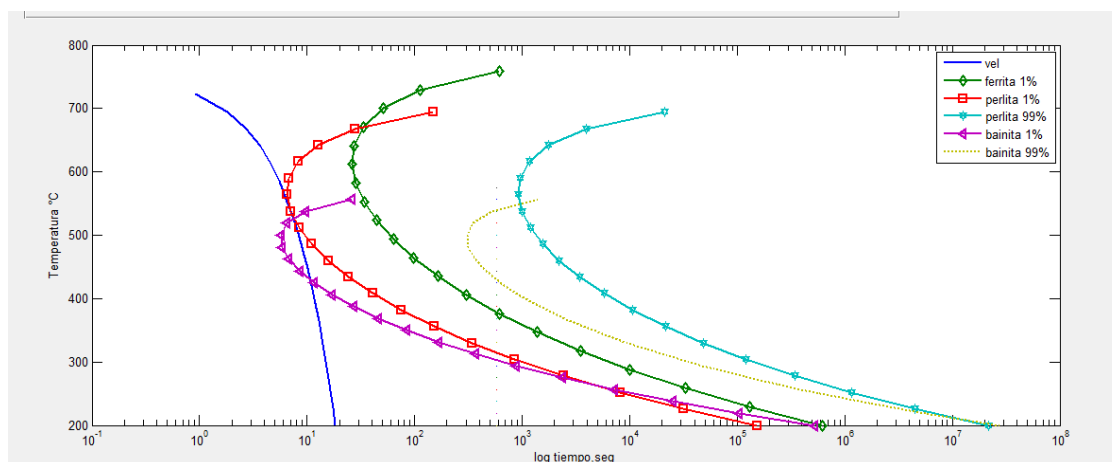


FIGURE 6. TTT DIAGRAM AS RESULT OF MATHEMATICAL MODELING BY JMARK EQUATIONS

When a compressive force has been applied before heat treatment, the starting temperature of phase transformation is decreased, the A1 and A3 temperatures decrease and TTT diagrams (temperature, time, transformation), make it run right, causing the bainite transformation is done faster, avoiding the formation of the nose establishing that the cooling is slower.

It is noted that in making this mathematical modeling bainite not be obtained, which could be tested experimentally, since only ferrite and pearlite was obtained. It was deduced that for bainite is necessary compression of the material hot.

To determine the residual stresses of the material, with the ANSYS® software satisfactory results were obtained, in which could show different strain may suffer material after completed the thermomechanical treatment, in this case the plastic and elastic deformation shown and Von Misses effort, this in order to complete the initial constitutive equation. Se the Fig. 7 to 16.

It is shown that depending on the amount of pearlite (purple) the material has a lower plastic deformation which makes the more impact resistant material, which may have increased if bainite been obtained experimentally.

It is noted that the low load applied pearlite formation is lower and increased the load also increases the formation of pearlite, but also if the load too low increases the percentage of it.

In the metallographics at loads 20 and 25 tons the plastic and elastic force are equal, because the percentage of pearlite in this material has the same percentage.

After the images obtained stress that were generated in the material , ANSYS ® keep the data of strain and stress experienced by the material when the solution element . This data is graphed in Excel where you could get Fig 17. Where can be seen in the beginning the elastic region, then the plastic deformation and in the end the breaking point. The Figure shown is for metallography suffered material 15ton load, this same procedure was developed for the other two loads.

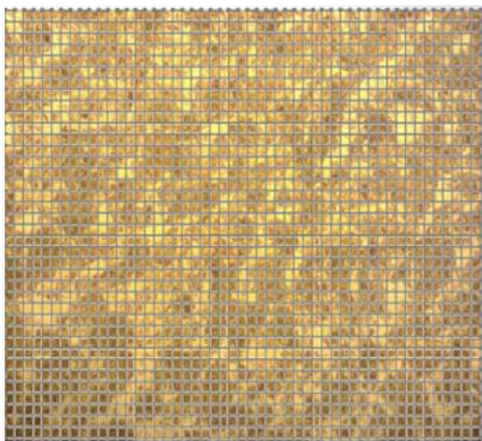


FIGURE 7. DIVIDE METALLOGRAPHY AT LOAD OF 15 TON

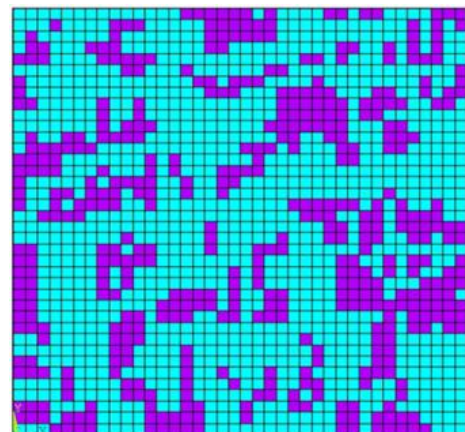


FIGURE 8. MODELLING METALLOGRAPHY AT LOAD OF 15 TONS AT ANSYS

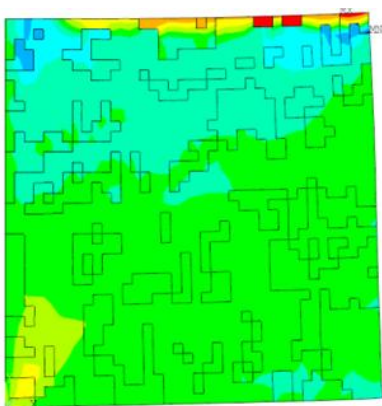


FIGURE 9. DIAGRAM OF ELASTIC DEFORMATION AT LOAD OF 15 TON

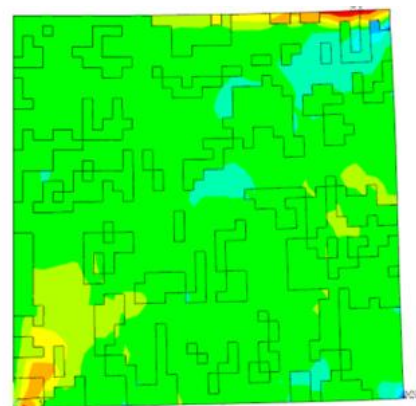


FIGURE 10. DIAGRAM OF PLASTIC DEFORMATION AT LOAD OF 15 TON

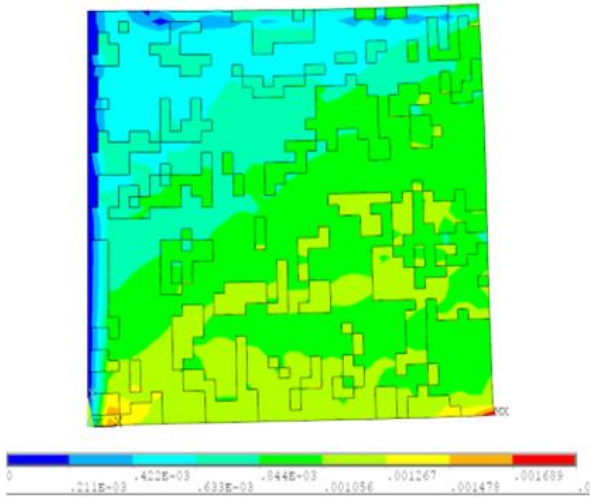


FIGURE 11. DIAGRAM OF VON MISSES STRESS AT LOAD OF 15 TON

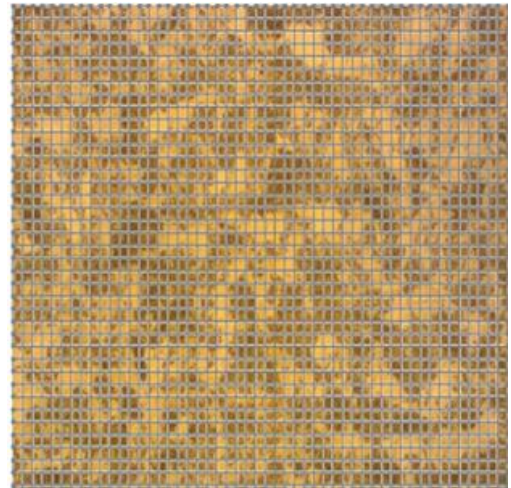


FIGURE 12. DIVIDE METALLOGRAPHY AT LOAD OF 20 TON

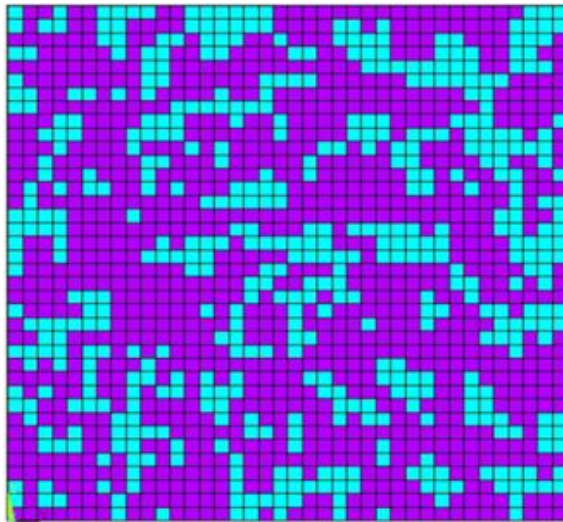


FIGURE 13. MODELLING METALLOGRAPHY AT LOAD OF 20 TONS AT ANSYS

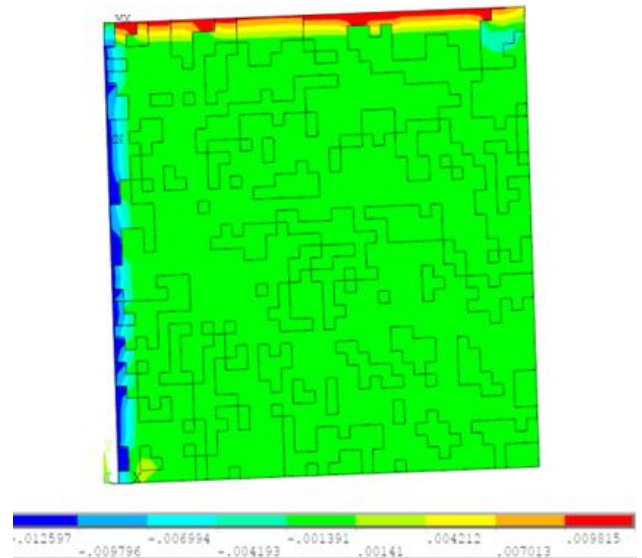


FIGURE 14. DIAGRAM OF ELASTIC DEFORMATION AT LOAD OF 20 TON

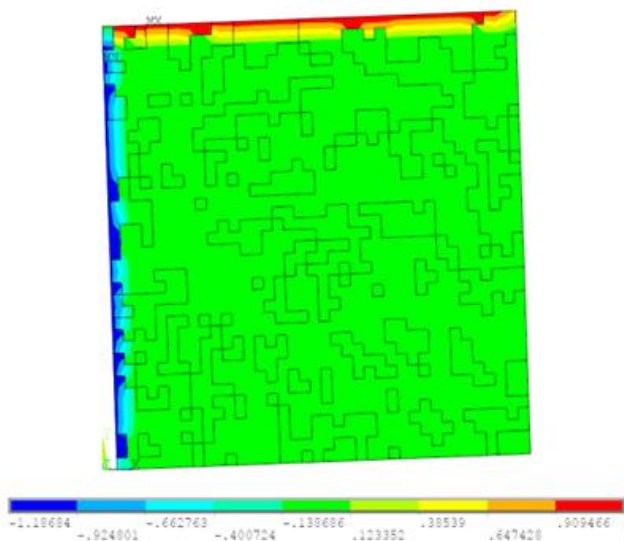


FIGURE 15. DIAGRAM OF PLASTIC DEFORMATION AT LOAD OF 20 TON

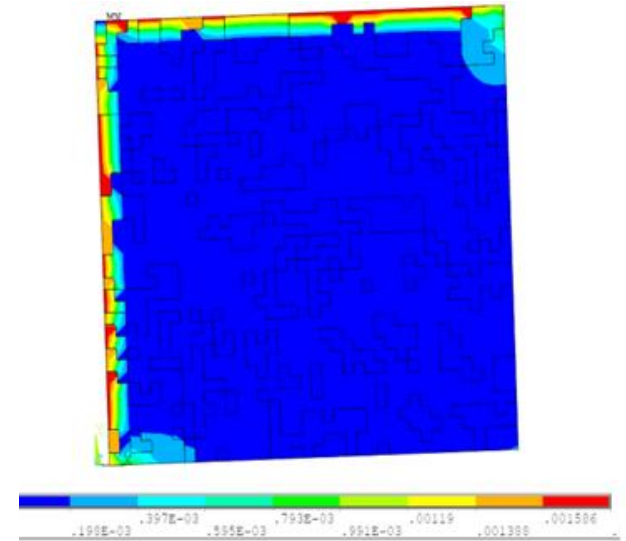


FIGURE 16. DIAGRAM OF VON MISSES STRESS AT LOAD OF 20 TON

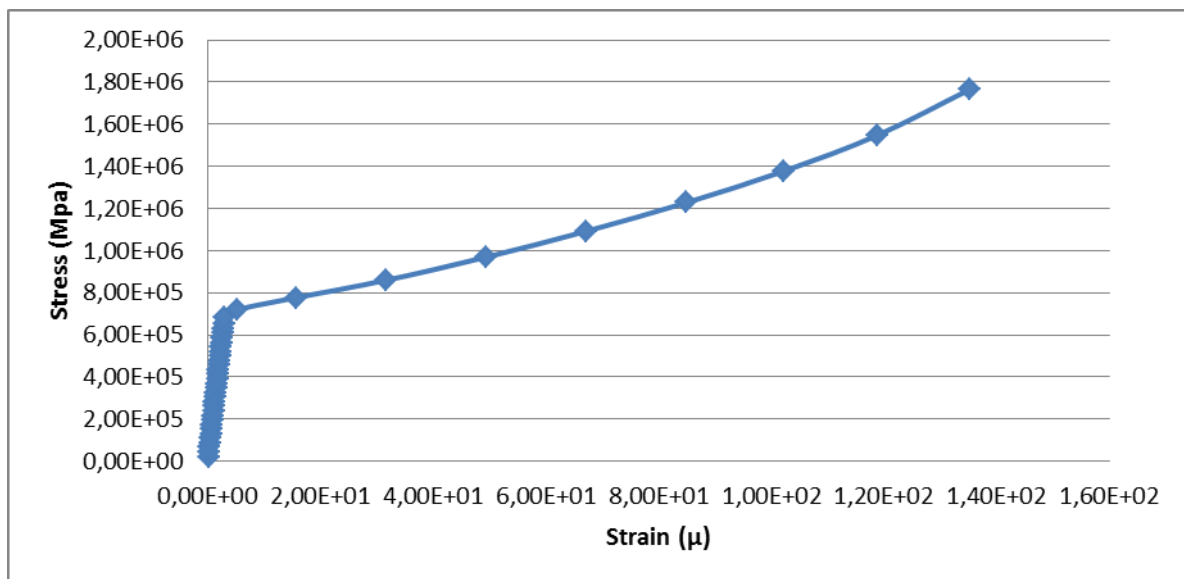


FIGURE 17. GRAPHIC STRESS VS. STRAIN AT LOAD OF 15 TON

IV. CONCLUSION

Mathematical modeling is a helpful tool to determine the optimization of processes in thermomechanical treatments. And without costly procedures to determine certain characteristics of steel as are the plastic and elastic deformation and Von Misses stress, it is important to know when required to do different processes of structural design which is one of the great applications this steel.

The comparison of the experimental part with the modeled is similar, which was the aim of this project is demonstrated that sufficient boundary conditions which made results were obtained optimum as if they had included more conditions were taken, the results they had not relevantly changed, but the process had been delayed to get.

Further research is recommended to perform modeling hot deformed to obtain bainite microstructure.

ACKNOWLEDGEMENTS

To carry out this research I want to thank my project manager Carlos Bohórquez, thanks to him I could learn everything you need. At the Free University for giving me teachers who helped build this project.

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