DETERMINATION OF THE CORRELATIONS BETWEEN A QUANTITATIVE CRITERION, EXPERIMENTAL EVIDENCE AND FINITE ELEMENT MODEL OF A POLYCRYSTALLINE SAMPLE OF CU-AL-BE UNDERGOING UNIAXIAL TENSION.

R. Lechuga-Taboada 1, F. N. García-Castillo 2, J. Cortés-Pérez 1
A. G. Lara-Rodríguez, A. Reyes-Solís

2Departamento de Materiales y Manufactura, DIMEI, Universidad Nacional Autónoma de México, Avenida Universidad 3000, Coyoacán, 04510 C. de México, México.

ABSTRACT

The martensitic transformation in Polycrystalline Shape Memory Alloys (PSMA) occurs in a much more complex way than in the monocrystalline case, this is due many factors affect the mechanical conditions in each grain, even between regions of the same grain. Besides the crystal orientation, the number and orientation of the neighbour grains are factors to affect the mechanical behaviour of each grain in the sample and in consequence, impacts in the formation of the variants who can appear, however the correlations between the variants formed in a grain and the local states of stress and strain that activate them are not established yet.

In this work a simulation in Finite Element Method (FEM) of PSMA sample is represented. The morphology of the grains was idealized like a hexagonal prism cluster in the central section of a PSMA of Cu-11.5%wtAl-0.6%wt Be undergoing uniaxial tension is presented. This model supposes only one layer of grains in his transverse section.

The topology of the model was based in a sample used in a previous work in which the crystalline orientation of several grains was reported [García, 2015].

In this work a simulation in Finite Element Method (FEM) of PSMA sample is represented. The morphology of the grains was idealized like a hexagonal prism cluster in the central section of a PSMA of Cu-11.5%wtAl-0.6%wt Be undergoing uniaxial tension is presented. This model supposes only one layer of grains in his transverse section. The topology of the model was based in a sample used in a previous work in which the crystalline orientation of several grains was reported [García, 2016].

Each hexagonal prism in the model poses a different crystal orientation but the same elastic constants. The FEM analysis considers only the elastic behaviour. This tensor can be obtained for nodes ubicated in different regions of the boundaries and centre zones of selected grains. That tensors are referred to each martensite variant (24 in the case of Cu-Al-Be) and the results was compared with experimental evidence and a quantitative criterion who selects the variants with most probability of appear, the variants who presents the highest values of maximum shear stress are compared with the variants predicted by this criterion and with the experimental evidence. The FEM analysis results shows how in several cases, the grain boundaries act like stress concentrators and, in some cases, the stress and strain tensor presents high variations in the value of his components trough the sections of grain boundary due to strong influence of the neighbours. This fact impacts in the activation of variants of martensite in each region of the grain.

KEYWORDS: POLICRYSTALLINE SHAPE MEMORY ALLOY, FINITE ELEMENT METHOD, STRESS INDUCED MARTENSITIC TRANSFORMATION, MARTENSITE VARIANTS.

INTRODUCTION

Currently the prediction of mechanical behaviour of polycrystalline materials is a hard problem because the elementary theory for single crystals is not directly applicable. The last is due to the boundary conditions of each grain are more complex than simple tension, even when the sample is hold to that condition. It’s known that parameters such Schmid Factor (SF) are widely used to predict the appariation of martensite variants in monocrystalline samples, but the prediction rate strongly decay in polycrystalline cases. That means that other factors affect the way of Stress Induced Martensitic Transformation (SIMT) occurs in the last case.

However, recently some authors [García, 2015] proposed a criterion to predict the martensite variants formed in polycrystalline shape memory material subject to simple tension. This criterion is based in a mathematical model [Cortés, 2007] and consider crystallographic aspects such the transformation system and crystalline orientation, besides parameters widely used un monocrystalline cases such SF and stress transformation diagram, besides consider a Strain Relation (SR). Where $\varepsilon_x$ is the deformation in rolling direction and $\varepsilon_y$ is the deformation in transversal direction in the strain tensor. [García, 2015]

Besides, many efforts have been done to simulate the mechanical behaviour in PSMA via FEM [Simonovsky, 2010]. However, the representation of grain shape and the topology of real sample still been a challenging issue for make good representation models.

In this work a comparation between a quantitative criterion [García, 2015] and FEM analysis in a quasi-bidimensional idealized polycrystalline sample has presented. The state of stress and strain of some nodes corresponding to a different grains and different zones in each grain are obtained and the
shear stress and \( SR \) in each base of transformation are calculated with the objective to predict which variants can occur in each grain before the martensitic transformation starts.

**MODEL CONSIDERATIONS**

The **FEM** model is based in a **PSME** of Cu–11.5% wt. Al–0.5% wt. Be. This sample was sample reported in a previous work [García, 2015], [García, 2016]. The elastic constants used in this work was reported by Ríos et al. [Ríos-Jara, 1991]. The load conditions are total restricted displacement in one side and constant displacement in “X” direction in the other side. The crystalline orientation of each grain reported is assigned to one hexagonal element, trying to maintain a similar topology to that of the observed sample.

![Figure 1: a) PSME sample. b) Idealized FEM sample. c) Grains undergoing stress martensitic transformation. d) FEM model topology.](image)

**RESULTS**

Stress and strain tensors of different nodes of the hexagonal prism corresponding to some grains (grain 23 as an example) are obtained, the tensors are referred to each transformation basis and the variants who present bigger values of shear stress and \( SR > 1 \) are considered like those that can be activated.

![Figure 2: a) Hexagonal element associated with grain 23. b) Grain 23 during SIMT. c) STD corresponding to grain 23. d) Projection of some martensite variants in observation basis.](image)

For each node of grain 23 considered in this work, the order of variants considered like possible active can change, however are always the same set of possible variants in different order. This set of variants are compared with the variants estimated by García [García, 2016].

<table>
<thead>
<tr>
<th>Variant estimated from FEM</th>
<th>( \tau_{xTyT} ) (MPa)</th>
<th>SR</th>
</tr>
</thead>
<tbody>
<tr>
<td>23</td>
<td>15.723</td>
<td>2.0938</td>
</tr>
<tr>
<td>9</td>
<td>16.9974</td>
<td>2.1716</td>
</tr>
<tr>
<td>16</td>
<td>12.7922</td>
<td>3.1674</td>
</tr>
<tr>
<td>5</td>
<td>9.4884</td>
<td>4.9499</td>
</tr>
<tr>
<td>3</td>
<td>24.3331</td>
<td>2.9978</td>
</tr>
</tbody>
</table>

*Table 1: Variants predicted from FEM analysis data in a node corresponding to hexagonal prism 23 (3,7,20 coincident with experimental evidence).*

**CONCLUSIONS**

Some variants predicted by García [García, 2016] are coincident with the variants estimated from FEM analysis but not all. The values of shear stress and \( SR \) can change in each node in a meaningful manner, but the variants that are consider like probably active are almost always the same in each hexagonal prism.

**REFERENCES**


**AKNOWLEDGEMENTS**

The authors express their gratitude to the PAPIIT program for the financial support through the UNAM-DGAPA-PAPIIT-IN115917, UNAM-DGAPA-PAPIME-PE-110018 projects and DGAPA for the postdoctoral fellowship awarded to F.N. García-Castillo.