MODELLING OF HYDROGEN EFFECTS ON THE THERMOMECHANICAL BEHAVIOUR OF NITI-BASED SHAPE MEMORY ALLOYS

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ABSTRACT

Nowadays, NiTi Shape Memory Alloys (SMAs) wires are subject to complex chemical loading in oral cavities. In the worst case, fractures are observed (see \cite{Yokoyama et al., 2001}). Hydrogen effects are suspected, by analogy with the hydrogen embrittlement well known in Ti alloy systems.

Accounting for effects of hydrogen diffusion on the NiTi SMA behaviour, a coupled chemo-thermo-mechanical constitutive model needs to be formulated. Based on the work of \cite{Lachiguer et al., 2016}, a first step consists in introducing material parameter dependencies (transformations temperatures, maximum transformation strain, hysteresis size …) to the normalized concentration of hydrogen in the NiTi constitutive law developed by \cite{Chemisky et al., 2011}.

The main limitation of this model is that the hydrogen concentration can only be considered as homogeneous. As nano-indentation tests reveal a heterogeneous distribution of hardness (which is indirectly related to the hydrogen concentration), it becomes necessary to take into account the gradient of hydrogen distribution from the surface to the cross section center. The temperature is also considered due to its influence on the mechanical response and the hydrogen diffusion.

To this end, we have to write the weak form of equilibrium equations for each field (thermal, mechanical and chemical fields) through a 2D domain. These equations are then discretized to be solved numerically by finite element method. We consider the case of a two dimensional plane stress element which has four nodes, with linear interpolation shape functions.

As explained before, the objective of this study is to develop a 2D finite element with three different fields. In the first part of this paper, we will describe and explain the main steps for the development of a special finite element with displacements, temperature and hydrogen concentration as degrees of freedom.

In the second part, we will discuss about the numerical results obtained with this element.

MODELING FORMULATION AND NUMERICAL RESOLUTION

The first step consists in taking into account all the physics phenomena that we suppose involved in the considered situation. We define three fields (thermal, mechanical and chemical) and write their corresponding equilibrium equations. After this, coupled behaviour laws are injected in the weak form of equilibrium equations. Thus we obtain the continuum form of the residue for each field and we get the forces term of the FE method. These equations are now discretized, by the finite element method depending on the adopted shape function.

We consider the case of a two dimensional plane stress element which has four nodes, four Degrees Of Freedom (DOF) and linear interpolation shape functions. The two first components are the displacement in the plane. The third and last components are respectively the temperature and the hydrogen concentration (see Figure 1).

For a given applied loading, composed of any of our field, residues become non-zero. The next steady state is found by modifying the internal variables in order to cancel the residue. To get a general approach, we choose a numerical resolution with the Newton-Raphson method. The computations of the derivative enable us to get the tangent stiffness matrix of the FE method.

INTRODUCTION

NiTi SMAs exhibit a martensitic transformation. It induces a recovery deformation at constant force widely considered for orthodontic treatments despite some fractures observed after few months in buccal cavity. A degradation of the mechanical properties of NiTi arches appears due to the presence of hydrogen. Indeed, the maximum strain decreases and the area of the hysteresis become smaller.

KEYWORDS: NiTi shape memory alloy, Hydrogen diffusion, Finite elements, Constitutive models, Orthodontic applications

Figure 1: Quadrangular finite element with four nodes and four DOF
The last step consists in sending to Abaqus the tangent stiffness matrix, the nodal forces vectors and all the internal variables. Figure 2 summarized the complete algorithm.

**NUMERICAL RESULTS**

The developed element described in the previous section is now tested. The chosen geometry is a square plate of 4 mm length. Thanks to the symmetries of the domain, we only study a quarter of the domain, discretized with 30 elements, in order to make possible the monitoring of the hydrogen diffusion every 0.2 mm.

A constant temperature of 40 °C is fixed for every node of the mesh, and some mechanical boundary conditions are applied to take into account the symmetries. Others boundary conditions are applied on the top of the plate. In a first step, a displacement of 0.0425 mm is prescribed and maintained. During the 2nd step, we applied a concentration of 0.01 ppm of hydrogen. Thirdly, we decrease the displacement until we return to the initial configuration. To finish, a displacement of 0.085 mm is applied then released. Figures 3 and 4 present the obtained results.

The figure 3 shows stress-strain curves. Due to the chemical boundary conditions and to the diffusion coefficient, top edge and center of the plate have not the same amount of hydrogen. The black curve corresponds to the same thermo-mechanical simulation without any chemical contribution.

Before the applying of chemical loading, there is no difference between the three curves. When we reach the 4.25 % of strain during the first mechanical loading, the diffusion begin.

The first unloading and second loading behaviors depend on the hydrogen concentration. Higher is the hydrogen quantities, smaller is the hysteresis area, which is the effect highlighted by [Lachiguer et al., 2016].

The figure 4 presents the hydrogen distribution. The diffusion coefficient was chosen in order to be in a transient state, so we have a heterogeneous concentration. The blue curve corresponds to the center and the black curve to the top edge. If we look to the time evolution of diffusion at the top side, a linear growth and after this an asymptotic convergence towards the imposed concentration is observed.

This numerical tool allows to access to the local information in a given material point with a given local hydrogen concentration (stress state, transformation state…). Such informations are mandatory for the design of SMA archwires considering the effect of hydrogen diffusion. As a prospect of this work, this formulation will be extended to take into account the effect of hydrogen on maximum strain, and in the longer term to a three dimensional element. The thermodynamic model of the coupling will also be completed and improved. The obtained numerical tool will allow analyzing of the effect of hydrogen diffusion on the performance of SMA-based orthodontic arches.

**REFERENCES**

