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Validation of Shape Memory Alloys Multiscale Modeling thanks to in-situ X-Rays Diffraction

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1. INTRODUCTION

The increasing use of Shape Memory Alloys (SMA) for complex applications requires a robust modeling of phenomena governing their behavior. The development of micro-macro multi-axial models is relevant since the SMA behavior is strongly correlated to appearance/disappearance/re-orientation of martensite variants at the microscale. Such approach relies the definition of transition scale rules, depending on the material microstructure, and an appropriate description of the behavior of constituents. On the other hand, it requires experiments for identification of parameters such as enthalpies or kinetic constants and validation of the model. This second point is addressed. A texturized nickel-titanium SMA (Ni_{49.95at%}Ti) is considered, exhibiting both martensitic and R-phase transformation. High temperature austenitic phase presents a body-cubic-centered unit cell (a₀=0.3015nm). The martensitic phase is monoclinic (a=0.2889nm; b=0.412nm; c=0.4662nm; β=96.8°) associated to 24 possible variants. The intermediate R-phase considered in the literature either orthorhombic or hexagonal [1] is taken hexagonal in this study (a_H=0.7345nm; c_H=0.5272nm) associated to 8 possible variants. In this paper a multiscale modeling able to model the multi-axial thermomechanical behavior of SMA is first presented. In situ X-Rays Diffraction (XRD) measurements are next performed under thermal or mechanical loading allowing us to quantify the volume fraction of each phase.

2. MULTISCALE MODEL DESCRIPTION [2]

The proposed multiscale model is relevant for multi-axial stress and thermal loading in a pseudo reversible framework [2]. The first scale involved for which mechanical and thermal quantities can be considered homogeneous is the variant scale. Indeed the model is based on the comparison of the free energies of each variant.

3.1 Energy balance

According to the thermomechanical coupling and neglecting the boundary effects, the free energy of a variant φ is given by eq. (1) where W_φ^T and W_φ^σ indicate the chemical energy (2) and elastic energy (3).

$$W_\varphi = W_\varphi^T + W_\varphi^\sigma \quad (1)$$

$$W_\varphi^T = H_\varphi - TS_\varphi \quad (2)$$

$$W_\varphi^\sigma = \frac{1}{2} \boldsymbol{\sigma}_\varphi : \mathbb{C}_\varphi^{-1} : \boldsymbol{\sigma}_\varphi \quad (3)$$

H_φ , S_φ are the variant specific enthalpy and entropy; T the temperature (K); $\boldsymbol{\sigma}_\varphi$ and \mathbb{C}_φ are the local stress and the stiffness tensor. The latter is considered uniform within the single crystal.

Calculation of associated volume fractions is made thanks to a Boltzmann probabilistic function so that the more probable variant is the one over the n possible variants minimizing the free energy. Volume fraction f_φ is given by:

$$f_\varphi = \frac{e^{-AW_\varphi}}{\sum_{\varphi=1}^n e^{-AW_\varphi}} \quad (4)$$

A is a parameter that introduces “inertial” effects ignored by the modeling.

3.2 Localization and homogenization rules

The intermediate scale is the single crystal scale. Determination of the stress at the variant scale requires a localization process combining Hill’s and Eschelby’s formulations. The variant is considered as an inclusion inside an equivalent medium. Its deformation $\boldsymbol{\varepsilon}_\varphi$ is given by:

$$\boldsymbol{\varepsilon}_\varphi = \mathbb{S}^E : \boldsymbol{\varepsilon}_\varphi^{tr} \quad (5)$$

\mathbb{S}^E is the Eschelby tensor that relies the variant strain $\boldsymbol{\varepsilon}_\varphi$ to its transformation “free” strain $\boldsymbol{\varepsilon}_\varphi^{tr}$. The latter only depends on the crystallographic parameters. Hill’s formulation is applied giving the local stress:

$$\boldsymbol{\sigma}_\varphi = \boldsymbol{\sigma}_g + \mathbb{C}_\varphi : (1 - \mathbb{S}^E) : (\boldsymbol{\varepsilon}_g^{tr} - \boldsymbol{\varepsilon}_\varphi^{tr}) \quad (6)$$

σ_g and ϵ_g^{tr} are the stress and transformation strain at the single crystal scale. Microstructure (fractions) is changing due to thermomechanical loading. The shape and distribution remain unknown. The Eshelby tensor cannot consequently be defined uniquely. A uniform strain hypothesis is thus assumed ($\mathcal{S}^E = 0$). A modulation of the stiffness tensor (7) is made thanks to δ coefficient ($0 < \delta < 1$) that takes the other inelastic phenomena into account [2]. Its introduction allows us to reduce the stress level generated by the uniform strain hypothesis.

$$\sigma_\varphi = \sigma_g + \delta \mathcal{C}_\varphi : (\epsilon_g^{tr} - \epsilon_\varphi^{tr}) \quad (7)$$

Averaging operations allow the calculation of the mean transformation strain (ϵ_g^{tr}) over the single crystal.

$$\epsilon_g^{tr} = \langle \epsilon_\varphi^{tr} \rangle = \sum_{\varphi=1}^n f_\varphi \epsilon_\varphi^{tr} \quad (8)$$

More classical homogenization and localization [3] schemes are used to link quantities defined at the single crystal scale to macroscopic quantities at the polycrystalline and final scale. It uses especially an orientation data file representative of the material obtained thanks to electron backscattered diffraction.

3. VALIDATION EXPERIMENTS

In situ X-Rays Diffraction (XRD) measurements are performed during tensile tests (figure 1.) and heating-cooling cycles (cooling in figure 2.) to validate the modeling. XRD permits monitoring of the average volume fraction of phases in presence. This operation requires the coupling of the multiscale model to a diffraction pattern model associated to the specific geometry of the diffraction apparatus. Experimental measurements gave key information on NiTi behavior in thermal case: transition temperatures, sequenced appearance of R-phase and martensite phase, hysteresis between heating and cooling... XRD measurements under applied stress give significantly different results since the R-phase does not appear as a precursor of martensite phase. The reason is that the transformation strain magnitude of R-phase is much lower than that of the martensite, reducing the chemo-mechanical coupling. We observe secondly that variants (of martensite) parallel to the loading direction are preferably selected during tensile test while the selection is uniform in case of thermal transformation. The model qualitatively allows us to simulate these specific points (results presented in the full paper). It also gives a good approximation of quantitative volume fraction evolution even if a better accordance may be obtained using true material parameters (entropies, enthalpies and transformation temperatures) instead of values taken from the literature [4].

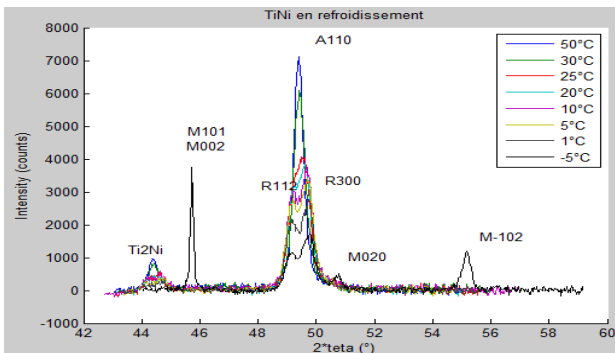


Figure 1. NiTi during cooling process*

*X-rays' source is Cobalt ($\lambda_{Co}=0.17853\text{nm}$). We can see the nucleation of R-phase (R) and martensite (M) activated planes from the principal $\{110\}$ austenite (A) plane.

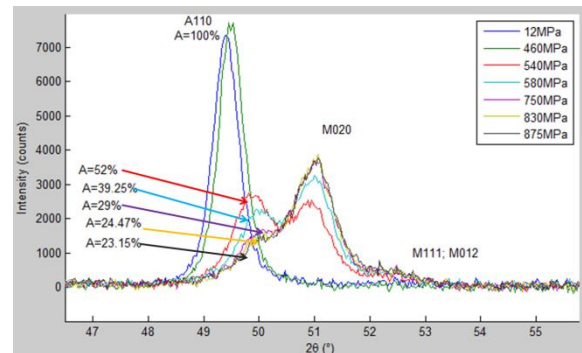


Figure 2. NiTi during tensile test*

4. SUMMARY AND CONCLUSION

A multiscale model is proposed able to model macroscopic quantities as deformation and microscopic quantities as volume fraction and orientation of R-phase and martensite variants as function of a macroscopic multiaxial thermomechanical loading. XRD measurements are shown to be an efficient way to validate the model estimation of local quantities. A good agreement is obtained between numerical and experimental results.

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