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# Finite element and experimental structural analysis of endodontic rotary file made of Cu-based single crystal SMA considering a micromechanical behavior model

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## Abstract

Shape Memory Alloys (SMAs) are widely used in endodontics as instruments for root canal preparation namely endodontic rotary files. Despite their high performances, compared to stainless steel instruments, it is still possible to enhance their cutting efficiency by acting on their shape and material properties. As an example, increasing the exhibited reversible martensitic transformation strain makes them more flexible without decreasing their mechanical strength. It becomes possible with single crystal SMAs. Cu-based (Cu-Al-Be, Cu-Zn-Al, Cu-Al-Mn) single crystal SMAs start emerging and can reach about 12% of martensitic transformation strain, in addition to their interesting antimicrobial properties. This study investigates, both numerically and experimentally, the development of endodontic files made of Cu-based single crystal SMAs. The numerical analysis is carried out by the finite element method. The geometry of the instrument is parameterized. Depending on the applied boundary conditions, bending, torsion, or combined bending-torsion loadings are represented. A micromechanical constitutive law is implemented in Abaqus via the UMAT subroutine to describe the thermomechanical behavior of the Cu-based single crystal SMA. Following the thus obtained numerical results, Coltene-Micromega company has manufactured endodontic file prototypes made of Cu-Al-Be sin-

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gle crystal SMA. A specific setup applying the same boundary conditions of torsion-bending loading, is used to characterize these SMA file prototypes. The good agreement between experimental and numerical responses, for a combined bending-torsion loading, proves the relevance of the proposed approach and the pertinence of considering Cu-based SMAs for endodontic file applications.

*Keywords:* Shape Memory Alloy, Endodontic files, Cu-based single crystal SMA, Finite element analysis, experimental analysis, combined bending-torsion

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## 1. Introduction

Root canal treatment is a dental procedure used to treat inflamed or/and infected tooth pulp. It enables a patient to retain a tooth in a healthy state on his dental arcade. The procedure is often complicated and, once the diagnosis is made, consists in isolating the tooth, opening the crown, shaping and cleaning the root canal, and finally filling it with a biocompatible sealer. To remove the dental pulp and its organo-mineral content, endodontic files are needed. The root canal preparation in endodontics relies on manual then rotary file capacity to remove organic content, microorganisms and predentin and to follow the curved areas while operating without causing any damage and any instrument failure. This capacity was mainly improved during the last decades. Manual stainless steel files were replaced by rotary ones with the same material making the root canal preparation more efficient and with fewer cases of failure. However, stainless steel rotary files had difficulties to follow the relatively curved and conical shape of the root canal for a given tooth. This curvature could have a circular arc shape or a plane/tridimensional “S” shape. This is due to their very weak exhibited reversible deformation induced by elasticity only. That is why endodontic rotary files made of NiTi SMAs emerged naturally as an interesting alternative to stainless steel ones (Pedrinha et al., 2018). In fact, SMAs and in particular NiTi alloys are able to deliver much higher reversible deformation thanks to the reversible martensitic transformation strain. It enables

22 the more flexible rotary file to better follow simple or double curved root canals  
23 during the preparation process. These properties allow the use of mechanized  
24 files driven in a rotation motion from generally 150 rpm to 350-600 rpm (Zelada  
25 et al., 2002; Padavala and Ganapathy, 2019). In addition, NiTi SMAs are also  
26 bio-compatible and show a good resistance to corrosion, a high strength stress  
27 and a high resistance to fatigue under bending and torsion loading (Shen et al.,  
28 2011; Jamleh et al., 2019). They have two main specific thermomechanical  
29 behaviors governed by forward and reverse martensitic phase transformation:  
30 superelasticity effect (SE) and shape memory effect (SME), with respectively  
31 a self recovering and a thermally assisted recovering of the martensitic trans-  
32 formation strain after unloading. The major available rotary endodontic files  
33 are SE even if SME ones, with more flexibility induced by martensite detwin-  
34 ning at quasi-constant buccal temperature, start to emerge and are known in  
35 endodontics as heat treated rotary files (Prados-Privado et al., 2019). However,  
36 continuously rotating NiTi files operate with the inherent risk associated with  
37 torque and cyclic fatigue failures. To decrease this risk, files were used in a  
38 mechanical reciprocating movement, turning a specific distance clockwise, then  
39 rotating counterclockwise (Karatas et al., 2016). Over the past years, a huge  
40 number of carried out research and development works enabled to enhance the  
41 cutting performances of these rotary files (Schaefer and Oitzinger, 2008). They  
42 acted on optimization of material parameters related to (SE) and (SME) mech-  
43 anisms, (Zinelis et al., 2007), on geometrical parameters as cross section shape,  
44 tip diameter, taper, pitch, operative length (Ahamed et al., 2018; Ha et al., 2017;  
45 De Arruda Santos et al., 2014; Arbab Chirani et al., 2011; Chevalier et al., 2018),  
46 and also on control parameters as speed rotation for continuous and reciprocating  
47 motion and maximum torsion torque. It has been determined that the tip  
48 diameter, the taper, and the cross section properties (shape, area and inertia),  
49 have in addition to SMA properties, an influence on the bending and torsion  
50 flexibilities (or stiffnesses) and on the torsion and fatigue resistance (Schäfer and  
51 Tepel, 1999; Rodrigues et al., 2016; Chi et al., 2017). The fatigue behavior of  
52 these NiTi SMA endodontic files and the corresponding induced fracture modes

53 were also investigated by (Ferreira et al., 2017; Aidasani et al., 2017) leading to  
54 the same conclusions. (Kim et al., 2012; McGuigan et al., 2013; Martins et al.,  
55 2017) showed that fracture while operating is induced by bending or torsion or  
56 both combined loading. Therefore, considering these results, rotating endodon-  
57 tic files performances were highly improved making more efficient, reproducible  
58 and safer the canal root preparation and reducing its duration. However, these  
59 improvements mainly focus on NiTi rotary files. Recently our research group  
60 showed that it is possible to even more improve performances of rotary files  
61 by considering Cu-based single crystal SMAs (Cu-SC-SMA) as for example the  
62 Cu-Al-Be alloy (Vincent et al., 2015, 2017). Using this SMA family should also  
63 contribute to the reduction of the root canal preparation time thanks to the  
64 antimicrobial properties of copper (Vincent et al., 2018). Copper is a powerful  
65 antimicrobial agent. Microorganisms survive only a few minutes on copper sur-  
66 faces (Grass et al., 2011; Prado et al., 2012) especially at 37°C and in conditions  
67 of 100% relative humidity (buccal conditions) (Ojeil et al., 2013). Associated  
68 with hydrogen peroxide, an endodontic irrigant, copper is able to kill bacte-  
69 ria in a very short time through the release of hydroxyl radicals (Hartemann  
70 et al., 1995). Conversely, sodium hypochlorite, the most widely used irrigation  
71 solution in endodontics, requires 60 minutes of contact time to eliminate mi-  
72 croorganisms (Spratt et al., 2001). Contrary to NiTi single crystals, it is easier  
73 to manufacture Cu-SC-SMA wires that are well adapted to process rotary files.  
74 Moreover, they have very interesting properties: (i) antimicrobial effect during  
75 root canal preparation and (ii) much higher flexibility induced by martensitic  
76 transformation strain that can go up to 12%. In addition, it is worth noting that  
77 polycrystal Cu-based SMAs present very high incompatibilities between grains  
78 inducing high internal stresses and fracture below low reversible transformation  
79 strains (about 3 or 4%) which also justifies the choice of Cu-SC-SMA.  
80 However, it has been shown that such Cu-SC-SMA wires, with a [1 0 0] crys-  
81 tallographic orientation in the axis direction, exhibit a very low transformation  
82 strain (low volume fraction of martensite) under torsion loading leading to an  
83 effective behavior close to the elastic one which is highly anisotropic. Therefore,

84 for given geometrical parameters, the obtained global response of the rotary en-  
85 dodontic instrument under torsion loading is stiffer than under bending loading  
86 (Sittner et al., 2003). Indeed, when the instrument rotation is hampered by  
87 the machined dentin, torsional loading occurs inducing the instrument failure.  
88 A part from it will then remain inside the root canal making it very difficult  
89 to eliminate. (Vincent et al., 2015) studied by the finite element method the  
90 influence of geometrical parameters on responses of Cu-SC-SMA rotary files sub-  
91 jected to bending and torsion loading following the Standard ISO-3630-1 (Int.  
92 Org. for Standardization, 2008). This study considers a macroscopic thermo-  
93 mechanical constitutive model proposed by (Peultier et al., 2006) and improved  
94 by (Chemisky et al., 2011). For this preliminary study, the adopted behavior  
95 model cannot accurately predict the specific torsional response of Cu-SC-SMA.  
96 In fact, the experimental analysis of the martensitic transformation process for  
97 these alloys, when subjected to torsion loading, shows an activation of very  
98 few martensite variants with a very low corresponding volume fraction (Tokuda  
99 et al., 1995; Bouvet et al., 2003; Casciati et al., 2007). It is related to the high  
100 incompatibility between martensite variants favorably oriented with respect to  
101 the torsion loading direction. It manifests through the moment-rotation global  
102 response with a high slope close to the elastic shear modulus and a very weak  
103 hysteresis size. Micromechanical models with crystalline plasticity-like formula-  
104 tion overcome such drawbacks of phenomenological behavior models. They de-  
105 scribe the thermomechanical behavior at the grain scale (each grain is assumed  
106 as a single crystal) by considering all potentially active variants of martensite.  
107 Each variant is characterized by a set of habit plane-twinning direction, and a  
108 volume fraction. Berveiller-Patoor’s research group proposed a micromechani-  
109 cal constitutive law based on this approach (Patoor et al., 1996). They derived  
110 a macroscopic model more adapted to polycrystalline Cu-based SMAs by ap-  
111 plying a self consistent scale transition technique to a Representative Volume  
112 Element (RVE) composed of a high number of grains. Each grain has a different  
113 crystallographic orientation related to the measured texture (Entemeyer et al.,  
114 2000). Other models considering the same approach are also available in liter-

115 ature and detailed in the review paper (Cissé et al., 2016). The single crystal  
116 version, initially proposed by (Patoor et al., 1996), improved by (Niclaeys et al.,  
117 2002; Merzouki et al., 2010; Collard and Ben Zineb, 2012) is implemented in  
118 the finite element code Abaqus. It well describes the martensite variant acti-  
119 vation in a Cu-based single crystal SMA, particularly for torsion loading. It is  
120 then more adapted to predict the torsional response of Cu-SC-SMA rotary files.  
121 Therefore, the present paper details the numerical analysis of rotary prototype  
122 made of Cu-SC-SMA considering the aforementioned micromechanical constitu-  
123 tive model. It is subjected to respectively bending, torsion and bending-torsion  
124 loading. The combined bending-torsion loading occurs on the instrument when  
125 it becomes difficult to shape the dentin; in that case, the instrument cannot  
126 freely rotate which adds the torsion sollicitation to the bending. The geometry  
127 of this rotary file is inspired from already used NiTi files and described with  
128 a CAD model developed with Catia<sup>®</sup> and exported to Abaqus<sup>®</sup>. It is meshed  
129 with a tetrahedral continuum solid element with quadratic interpolation. The  
130 applied boundary conditions and loading respect the recommendation of the  
131 ISO Standard 3630-1, (Int. Org. for Standardization, 2008). The identification  
132 of the material parameters and the qualification of obtained numerical results  
133 rely on experimental results carried out using a specific setup (Xolin et al.,  
134 2020). It allows to apply bending and torsion loading in combined or separated  
135 ways. Prototypes are processed by Coltene-Micromega<sup>®</sup> using Cu-SC-SMA  
136 wires manufactured by Nimesis<sup>®</sup>. The obtained numerical results correctly cor-  
137 relate with experimental results and prove the following original features: (i)  
138 finite element analysis considering micromechanical constitutive law predicts  
139 in a more accurate way the response in torsion of rotary files made of Cu-SC-  
140 SMA, (ii) combining bending with torsion for these rotary files reduces their  
141 torsional stiffness and then moderates the aforementioned torsional response  
142 weakness, (iii) considering the interesting antimicrobial properties of Cu and  
143 despite this torsional response weakness, it should be possible to develop new  
144 and innovative versions of rotary files made of Cu-SC-SMA. In fact, it shows  
145 that responses of Cu-SC-SMA rotary endodontic files are close to the ones of

146 commercial instruments made of NiTi. This is true for both separated and com-  
147 bined bending-torsion loadings. Indeed, obtained values of rotations and their  
148 induced moments are in the same range as what is measured for commercial  
149 instruments. Furthermore, the analysis of sensitivity to geometrical parameters  
150 also leads to the same tendencies for commercial instruments (Gavini et al.,  
151 2018).

152 The present paper is organized as follows: after the introduction, section 2  
153 details the finite element numerical model with geometry, meshing, boundary  
154 conditions, loading cases and the adopted micromechanical constitutive model  
155 and its implementation in the finite element code Abaqus<sup>®</sup>. Section 3 presents  
156 the experimental testing device and the Cu-SC-SMA prototypes. Differential  
157 Scanning Calorimetry (DSC), tensile, bending, torsion and combined bending-  
158 torsion tests are performed to identify the material parameters of the microme-  
159 chanical constitutive model describing the Cu-SC-SMA thermomechanical be-  
160 havior. Bending, torsion and combined bending-torsion loadings are applied to  
161 validate the proposed model. Section 4 presents the adopted Taguchi design of  
162 experiment (DOE) in order to determine the influence of geometrical parame-  
163 ters on the equivalent response in combined bending-torsion loading. Section  
164 5 presents an overall discussion of the obtained results. The last section gives  
165 some conclusions and prospects.

## 166 **2. Finite element response analysis of the rotary endodontic file** 167 **made of Cu-SC-SMA**

### 168 *2.1. Introduction*

169 The proposed finite element analysis aims at predicting the global response  
170 of the proposed rotary endodontic file made of Cu-SC-SMA and to analyze the  
171 corresponding local state, at each material point, in terms of stresses, strains,  
172 activated martensite variants and their corresponding volume fractions. The  
173 adopted geometrical model is parameterized allowing to analyze the sensitiv-  
174 ity of the rotary file response to the geometrical parameters. Applied boundary



175 conditions are consistent with the ISO Standard 3630-1 ([Int. Org. for Standard-](#)  
 176 [ization, 2008](#)). They induce a bending-torsion loading applied in combined or  
 177 separated ways. The geometry is meshed with tetrahedral continuum elements  
 178 and a mesh refinement convergence is carried out. A micromechanical consti-  
 179 tutive model describes the thermomechanical behavior of the Cu-based single  
 180 crystal SMA. This finite element analysis allows to predict the effect of the tor-  
 181 sion on the global bending-torsion response of the studied rotary endodontic  
 182 files.

### 183 2.2. Geometry, mesh, boundary conditions and loading

184 The studied Cu-SC-SMA endodontic file presents a parameterized geometry  
 185 defined by figure 1. It presents a cylindrical part characterized by its diameter  
 186 and a tapered helical part characterized by its cross-section shape, its length,  
 187 its taper, its constant or variable pitch and its tip diameter. The variation  
 188 of these geometrical parameters allows to analyze their effects on the global  
 189 bending-torsion response. For each set of geometrical parameters, the CAD  
 190 software CATIA<sup>®</sup> generates the corresponding instrument geometry which is  
 exported into the finite element code Abaqus<sup>®</sup>. Then the meshing process

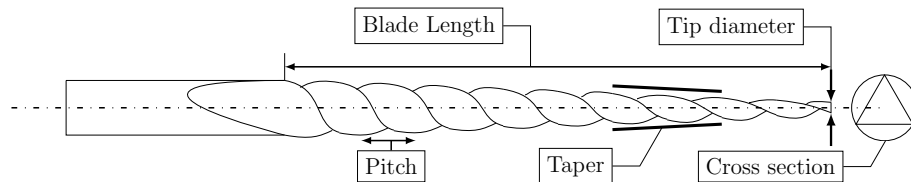


Figure 1: Parametrized geometry of a studied rotary endodontic file.

191  
 192 is applied. It considers tetrahedral continuum elements with 10 nodes using  
 193 quadratic interpolation (labeled in Abaqus<sup>®</sup> C3D10) and a given number of  
 194 intervals of variable size in each edge. This size takes into account the evolution  
 195 of the stress state and a predicted area of the martensitic transformation under  
 196 bending-torsion loading. Figure 2 presents an example of the obtained mesh for  
 197 the helical part after taking into account the assigned geometrical values and  
 198 the convergence of the refinement mesh process. It leads to a model with 21 500

elements. Regarding the boundary conditions, a part of the instrument with

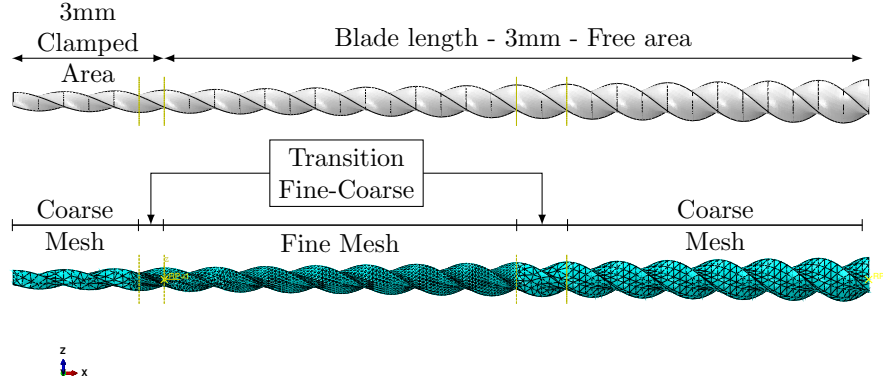


Figure 2: Example of obtained mesh for the helical part of the instrument.

199

200 a 3 mm length starting from its tip is clamped. Two rotations corresponding  
 201 to bending and torsion are applied in two reference points as depicted in figure  
 202 3. This leads to three loading cases: torsion, bending and combined torsion-  
 203 bending. As the instrument is generally rotating with a constant speed, the  
 204 analysis assumes a quasi-static loading. Also note that the boundary conditions  
 205 can be applied to any wire or prototype instrument with different cross-section  
 206 shape, diameter, taper and pitch length.

207 *2.3. Micromechanical constitutive law for Cu-SC-SMA and its implementation*  
 208 *in a finite element code*

209 The thermomechanical behavior of the Cu-SC-SMA is described by a con-  
 210 stitutive model, developed by (Patoor et al., 1996), and (Niclaeys et al., 2002).  
 211 Its implementation in Abaqus via the subroutine UMAT, initially undertaken  
 212 by (Merzouki et al., 2010; Collard and Ben Zineb, 2012), is deeply redrafted in  
 213 this work leading to an updated version enhancing the convergence process and  
 214 reducing computation CPU time. It is based on a crystalline plasticity-like ap-  
 215 proach and describes the activation of martensite variants in the crystalline  
 216 lattice and its effect on the macroscopic thermomechanical behavior. This

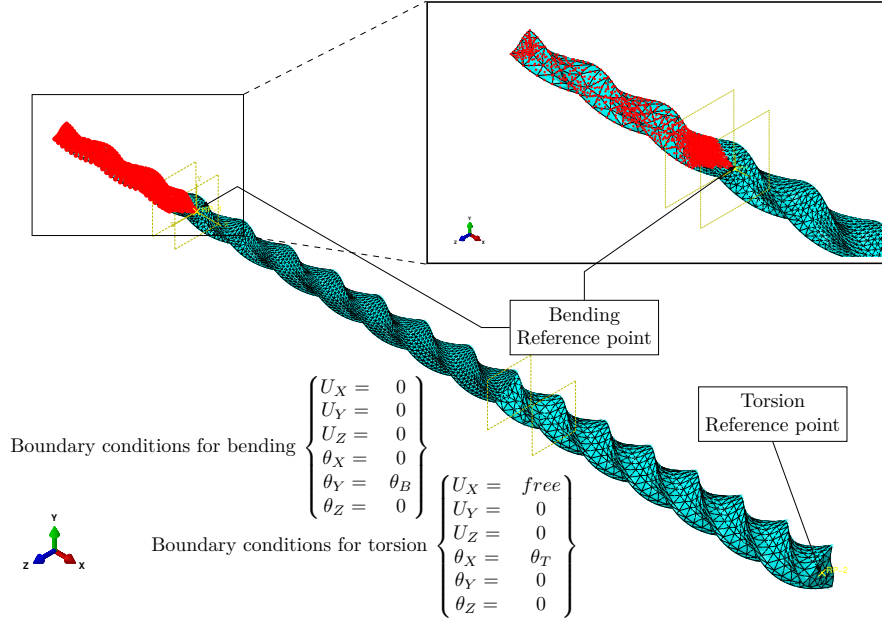


Figure 3: Applied boundary conditions for bending and torsion.

217 model presents 24 scalar internal variables corresponding to volume fractions  
 218 of martensite variants. Each variant is defined with a set of two vectors. One  
 219 is normal to the given habit plane,  $\vec{n}$ , whereas the other defines the twinning  
 220 direction,  $\vec{m}$ , table 1 and figure 4. They are expressed in the local coordinate  
 221 system of the single crystal. A rotation matrix defines the orientation of the  
 222 local coordinate system, related to the single crystal, with respect to the global  
 223 coordinate system. It characterizes the single crystal lattice orientation. The  
 224 intrinsic transformation strain  $\tilde{\varepsilon}_{ij}^n$  for any martensite variant ( $n$ ) depends on  
 225 their two vectors  $\vec{n}^n$  and  $\vec{m}^n$  and a constant transformation amplitude  $g$  as  
 226 follows:

$$\tilde{\varepsilon}_{ij}^n = \frac{1}{2}g(m_i^n n_j^n + m_j^n n_i^n) = \frac{1}{2}gR_{ij}^n \quad (1)$$

227 where  $R^n$  is the symmetric part of the Schmid tensor for the variant ( $n$ ). In the  
 228 case of multi-variants simultaneously active, the global transformation strain  
 229 is the resultant of all active variant transformation strains weighted by their

Table 1: Values of  $\vec{n}$  and  $\vec{m}$  for Cu-Al-Be single crystal SMA .

Variant	$n_1$	$n_2$	$n_3$	$m_1$	$m_2$	$m_3$
1	-0.168	0.688	0.705	-0.121	-0.725	0.678
2	-0.168	0.705	0.688	-0.121	0.678	-0.725
3	0.168	0.688	0.705	0.121	-0.725	0.678
4	0.168	0.705	0.688	0.121	0.678	-0.725
5	-0.688	-0.168	0.705	0.725	-0.121	0.678
6	-0.705	-0.168	0.688	-0.678	-0.121	-0.725
7	-0.688	0.168	0.705	0.725	0.121	0.678
8	-0.705	0.168	0.688	-0.678	0.121	-0.725
9	-0.168	-0.688	0.705	-0.121	0.725	0.678
10	-0.168	-0.705	0.688	-0.121	-0.678	-0.725
11	0.168	-0.688	0.705	0.121	0.725	0.678
12	0.168	-0.705	0.688	0.121	-0.678	-0.725
13	0.705	-0.168	0.688	0.678	-0.121	-0.725
14	0.688	-0.168	0.705	-0.725	-0.121	0.678
15	0.705	0.168	0.688	0.678	0.121	-0.725
16	0.688	0.168	0.705	-0.725	0.121	0.678
17	0.688	-0.705	0.168	-0.725	-0.678	0.121
18	0.705	-0.688	0.168	0.678	0.725	0.121
19	-0.688	0.705	0.168	0.725	0.678	0.121
20	-0.705	0.688	0.168	-0.678	-0.725	0.121
21	-0.705	-0.688	0.168	-0.678	0.725	0.121
22	-0.688	-0.705	0.168	0.725	-0.678	0.121
23	0.705	0.688	0.168	0.678	-0.725	0.121
24	0.688	0.705	0.168	-0.725	0.678	0.121

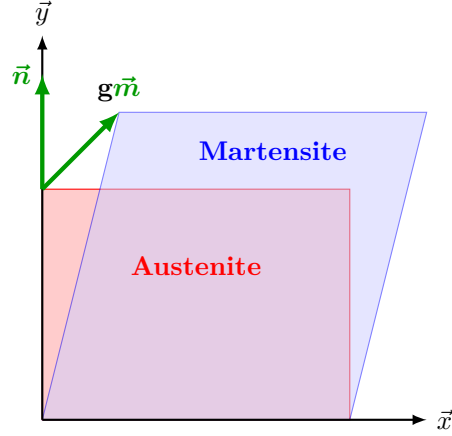


Figure 4: Definition of Habit plane and twinning direction where  $\vec{n}$ ,  $\vec{m}$  and  $g$  are the normal of the habit plane, the twinning direction and the transformation displacement respectively.

230 respective volume fractions ( $f^n = \frac{V_n}{V_{RVE}}$ ) as follows:

$$\varepsilon_{ij}^{tr} = \sum_n \tilde{\varepsilon}_{ij}^n f^n \quad (2)$$

231 where  $V_n$  is the volume occupied by the variant  $n$  and  $V_{RVE}$  is the total volume  
 232 of the Representative Volume Element (RVE) characterizing a given material  
 233 point. The phase transformation process is then characterized by the volume  
 234 fraction of the 24 variants assumed as internal variables. These volume fractions  
 235 are constrained by martensitic transformation saturation leading to  $0 \leq f^n \leq 1$   
 236 and  $\sum_n f^n \leq 1$ . By considering the defined global transformation strain in  
 237 addition to the classical elastic and thermal expansion strains, and applying  
 238 the first principle of thermodynamics, the micromechanical constitutive model  
 239 derives from the following assumed expression of the Gibbs free energy expressed  
 240 at the lattice scale:

$$\Delta G(\boldsymbol{\sigma}, T, f^n) = \sigma_{ij} \varepsilon_{ij} - W_{elas} - \Delta G_{ch} - W_{inter} \quad (3)$$

241 where  $\boldsymbol{\sigma}$ ,  $\boldsymbol{\varepsilon}$  and  $T$  are respectively the stress and strain tensors and the tem-  
 242 perature, in a material point, and where  $W_{elas}$ ,  $\Delta G_{ch}$ ,  $W_{inter}$  are respectively  
 243 the elastic energy, the chemical energy variation between the austenitic and

244 martensitic phases and the interface energy. This interface energy is assumed  
 245 negligible due to the flat shape of martensite variants. After some intermedi-  
 246 ate developments detailed in (Siredey et al., 1999), the final expression of the  
 247 Gibbs free energy is depicted by equation (4), where  $\alpha$ ,  $\delta_{ij}$ ,  $T_0$ ,  $T_I$  and  $B$  are  
 248 the thermal expansion coefficient, the Kröneckers symbol, the thermodynamic  
 249 temperature equilibrium between austenitic and martensitic phases, the initial  
 250 temperature of the material and the chemical energy respectively.

$$\begin{aligned} \Delta G(\boldsymbol{\sigma}, T, f^n) = & \frac{1}{2} \sigma_{ij} \mathbb{S}_{ijkl} \sigma_{kl} + \sigma_{ij} \varepsilon_{ij}^{tr} + \alpha \delta_{ij} (T - T_I) \sigma_{ij} \\ & + B(T - T_0) \sum_n f^n - \frac{1}{2} \sum_{n,m} f^n H^{nm} f^m \end{aligned} \quad (4)$$

251 The total energy  $\boldsymbol{\sigma} : \boldsymbol{\varepsilon}$  is split into an elastic part, a transformation part related  
 252 to the transformation strain  $\boldsymbol{\varepsilon}^{tr}$  and a thermal expansion part related to the  
 253 expansion tensor. The expansion tensor is assumed isotropic and controlled by  
 254 the scalar  $\alpha$ . The elastic energy is expressed as a function of the stress tensor  
 255 and the fourth order elasticity tensor  $\mathbb{S}$ . The chemical energy linearly depends  
 256 on the temperature variation and volume fraction of variants. The last term in  
 257 equation (4) represents the interaction energy related to internal stresses. It is  
 258 induced by incompatibilities between martensite variants. In order to simplify  
 259 equations, the interaction between each variant is represented in a matrix  $H^{nm}$   
 260 given in table 2. It lists the compatibilities and incompatibilities between all  
 261 variants. Taking into account the constraints on the volume fraction of each  
 262 variant modifies the expression of Gibbs energy and adds the following terms :

$$\psi_{const} = \sum_n \lambda_1^n f^n + \lambda (1 - \sum_n f^n) \quad (5)$$

It leads to the following expression of the Lagrangian:

$$\begin{aligned} \mathcal{L} = & \sigma_{ij} \varepsilon_{ij} - \Delta G_{ch} - W_{elas} - W_{inter} - \psi_{const} \\ = & \frac{1}{2} \sigma_{ij} \mathbb{S}_{ijkl} \sigma_{kl} + \sigma_{ij} \varepsilon_{ij}^{tr} + \alpha \delta_{ij} (T - T_I) \sigma_{ij} - B(T - T_0) \sum_n f^n \\ & - \frac{1}{2} \sum_{n,m} f^n H^{nm} f^m - (\sum_n \lambda_1^n f^n + \lambda (1 - \sum_n f^n)) \end{aligned} \quad (6)$$

Table 2: Interaction matrix describing compatibilities (C) and incompatibilities (I) between variants.

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
1	C	C	C	C	I	I	C	I	C	I	C	I	I	C	I	I	I	I	I	C	C	I	I	I
2	C	C	C	C	I	I	I	C	I	C	I	C	C	I	I	I	I	I	C	I	I	C	I	I
3	C	C	C	C	C	I	I	I	C	I	C	I	I	I	I	C	I	C	I	I	I	I	C	I
4	C	C	C	C	I	C	I	I	I	C	I	C	I	I	C	I	C	I	I	I	I	I	I	C
5					C	C	C	C	C	I	I	I	I	C	I	C	C	I	I	I	I	C	I	I
6					C	C	C	C	I	C	I	I	C	I	C	I	I	C	I	I	C	I	I	I
7					C	C	C	C	I	I	C	I	I	C	I	C	I	I	C	I	I	I	I	C
8					C	C	C	C	I	I	I	C	C	I	C	I	I	I	I	C	I	I	C	I
9									C	C	C	C	I	I	I	C	I	I	I	C	C	I	I	I
10									C	C	C	C	I	I	C	I	I	I	C	I	I	C	I	I
11									C	C	C	C	I	C	I	I	I	C	I	I	I	I	C	I
12									C	C	C	C	C	I	I	I	C	I	I	I	I	I	I	C
13													C	C	C	C	I	C	I	I	C	I	I	I
14													C	C	C	C	C	I	I	I	I	C	I	I
15													C	C	C	C	I	I	I	C	I	I	C	I
16													C	C	C	C	I	I	C	I	I	I	I	C
17																	C	C	C	C	I	C	I	C
18																	C	C	C	C	C	I	C	I
19																	C	C	C	C	I	C	I	C
20																	C	C	C	C	C	I	C	I
21																					C	C	C	C
22																					C	C	C	C
23																					C	C	C	C
24																					C	C	C	C

263 where  $\lambda_1^n$  and  $\lambda$  are Lagrangian multipliers allowing to ensure the transforma-  
 264 tion saturation conditions. The application of the Clausius-Duhem condition  
 265 integrating the expression of the Lagrangian  $\mathcal{L}$  leads to the decomposition of  
 266 strains and expressions of driving forces for martensite variants:

$$\left( \underbrace{\left( \left( \frac{\partial \mathcal{L}}{\partial \boldsymbol{\sigma}} - \boldsymbol{\varepsilon} \right) : \dot{\boldsymbol{\sigma}} + \frac{\partial \mathcal{L}}{\partial T} \dot{T} + \sum_n \left( \frac{\partial \mathcal{L}}{\partial f^n} \dot{f}^n + \frac{\partial \mathcal{L}}{\partial \lambda_1^n} \dot{\lambda}_1^n \right) + \frac{\partial \mathcal{L}}{\partial \lambda} \dot{\lambda} \right)}_{\dot{\mathcal{L}}} \right) \geq 0 \quad (7)$$

$$\left( -S^{RVE} \dot{T} - \vec{q} \cdot \frac{\vec{grad} T}{T} \right)$$

267 where  $S^{RVE}$  is the entropy of the RVE,  $\vec{q}$  is the heat flux induced by dissipation  
 268 and  $T$  the current temperature of the RVE. Dot over symbols represent their  
 269 rate form. Equation (7) leads to the following equations:

$$\begin{cases} \mathbb{S}_{ijkl} \sigma_{kl} + \alpha \delta_{ij} (T - T_I) + \varepsilon_{ij}^{tr} - \varepsilon_{ij} = 0 \\ -B \sum_n f^n - S^{RVE} = 0 \\ g \sigma_{ij} R_{ij}^n - B(T - T_0) e^n - \sum_m H^{nm} f^m - \lambda_1^n + \lambda e^n = F_{yield}^n \end{cases} \quad (8)$$

270 where  $(e^1, \dots, e^k)$  is a basis of  $\mathbb{R}^k$  defined as  $e_i^n = \begin{cases} 0 & \text{if } i \neq n \\ 1 & \text{if } i = n \end{cases}$ .

271 The two first driving forces are equal to zero because they correspond to ther-  
 272 moelasticity occurring without dissipation whereas the third driving force is  
 273 related to phase transformation occurring with dissipation. This justifies the  
 274 introduction of a yield force  $F_{yield}^n$  associated to each active variant ( $n$ ) taking  
 275 a different value during forward and reverse transformation. The temperature  
 276 gradient term becomes equal to zero by assuming a uniform temperature in the  
 277 whole RVE. Combining equations (8) and their rate form allows to determine  
 278 the rate of volume fraction of martensite  $\dot{f}^n$  for each active variant ( $n$ ) which  
 279 reads:

$$\dot{f}^n = \sum_m \hat{H}_{nm}^{-1} \left[ \tilde{\varepsilon}_{ij}^m \mathbb{C}_{ijkl} \dot{\varepsilon}_{kl} - \left( \tilde{\varepsilon}_{pq}^m \mathbb{C}_{pqrs} \alpha_{rs} + B e^m \right) \dot{T} \right] \quad (9)$$

280 where the fourth order tensor  $\mathbb{C} = \mathbb{S}^{-1}$  is the elasticity tensor and  $\hat{H}_{nm} =$   
 281  $\left( H^{nm} + \tilde{\varepsilon}_{ij}^n \mathbb{C}_{ijkl} \tilde{\varepsilon}_{kl}^m \right)$  is a  $k^v \times k^v$  reversible matrix where  $k^v$  is the number of



282 active variants. Combining the rate form of equations (8) and (9) allows to de-  
 283 rive the rate form of the micromechanical based thermomechanical constitutive  
 284 equations for the Cu-Al-Be single crystal SMA that reads:

$$\dot{\sigma}_{ij} = l_{ijkl}\dot{\epsilon}_{kl} - m_{ij}\dot{T} \quad (10)$$

$$\text{where } \begin{cases} l_{ijkl} = \mathbb{C}_{ijkl} - \sum_{n,m} \mathbb{C}_{ijrs} \tilde{\epsilon}_{rs}^n \hat{H}_{nm}^{-1} \tilde{\epsilon}_{pq}^m \mathbb{C}_{pqkl} \\ m_{ij} = \mathbb{C}_{ijkl} \alpha \delta_{kl} - \sum_{n,m} \mathbb{C}_{ijrs} \tilde{\epsilon}_{rs}^n \hat{H}_{nm}^{-1} (B e^m + \tilde{\epsilon}_{pq}^m \mathbb{C}_{pqkl} \alpha \delta_{kl}) \end{cases}$$

285 These constitutive equations are solved with an iterative method based on the  
 286 return mapping approach. The obtained numerical tool is implemented in  
 287 Abaqus<sup>®</sup> via the subroutine UMAT. The numerical resolution is detailed in  
 288 (Collard and Ben Zineb, 2012). The implementation process in Abaqus via  
 289 the subroutine UMAT is initially carried out in (Merzouki et al., 2010). It is  
 290 redrafted in a deep way in this work enabling to enhance the convergence pro-  
 291 cess and to reduce the computation CPU time. This behavior model presents  
 292 metallurgical parameters as transformation temperatures and crystallographic  
 293 characteristics as lattice orientation and habit plane and transformation direc-  
 294 tion for all variants. It also needs to identify phenomenological parameters as  
 295 the elastic coefficients, the compatibility and incompatibility coefficients, the  
 296 transformation amplitude  $g$  and the yield forces for each variant  $n$ ,  $F_{yield}^n$ . Re-  
 297 sults issued from this finite element analysis are compared to the ones obtained  
 298 experimentally. The experimental protocol is detailed in the next section.

### 299 **3. Experimental response analysis of the rotary endodontic file made** 300 **of Cu-SC-SMA**

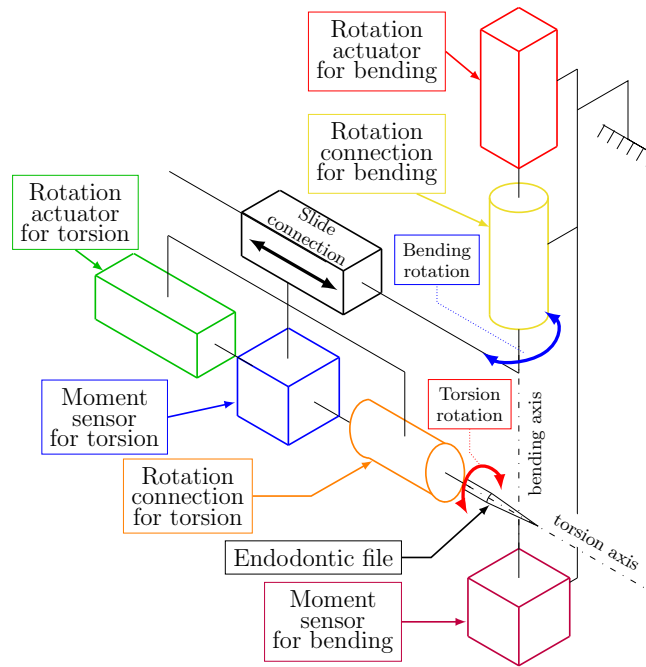
301 The experimental part of this study has a double objective: (i) the identifi-  
 302 cation of material parameters and (ii) the validation of the FE based numerical  
 303 approach developed in the previous section. In this section, the testing device for  
 304 combined bending torsion loadings is briefly presented, then the experimental  
 305 protocol is detailed.

306 *3.1. Experimental setup for combined bending-torsion loading*

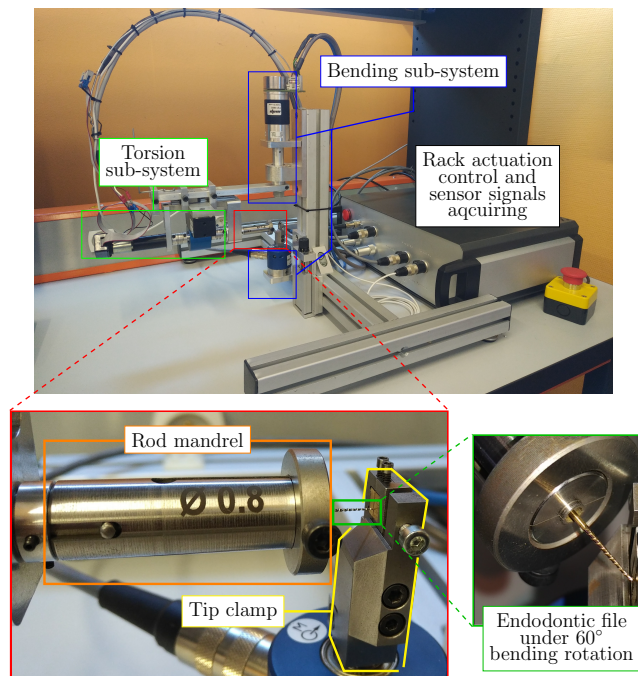
307 The experimental testing device is designed to study the bending and torsion  
308 responses of endodontic files under bending, torsion or combined bending-torsion  
309 loadings. It is based on the standard ISO 3630-1 ([Int. Org. for Standardiza-](#)  
310 [tion, 2008](#)). The main goal of these tests on endodontic file is to determine  
311 its flexibility and its resistance to torsional and bending loadings. Indeed, a  
312 bending loading is applied on the endodontic file when it has to follow the path  
313 of a curved root canal, and a torsion loading is applied due to the continuous  
314 rotation movement which allows the file to progress inside the narrow root canal  
315 and shape it. However, both bending and torsion loadings applied on the en-  
316 dodontic file are combined during the endodontic treatment and represent the  
317 most severe loading case. The considered testing device is able to measure the  
318 bending, torsion and combined bending-torsion loadings. It is composed as two  
319 subsystems: (i) a subsystem for torsion and (ii) a subsystem for bending. The  
320 kinematic principle and a detailed picture of the testing device are depicted by  
321 figures [5a](#) and [5b](#) respectively. The endodontic file is clamped 3 mm from its  
322 tip end and on its rod end 17 mm from the tip. It is loaded in torsion and  
323 bending by two rotation actuators. The first rotation is applied around the  
324 endodontic file axis whereas the second is applied around an axis perpendicular  
325 to this latter. Two corresponding sensors are associated to these actuators in  
326 order to measure induced moments. This testing device allows to apply an up  
327 to 60° rotation amplitude with 30 N.mm measured torque in bending and 20  
328 N.mm torque with no limitation rotation in torsion. Figure [6](#) shows the possible  
329 applied loading paths of bending or torsion (figure [6a](#)) and combined bending-  
330 torsion (figure [6b](#)). ([Xolin et al., 2020](#)) gives more details about this testing  
331 device.

332 *3.2. Material parameter identification with Cu-SC-SMA wire*

333 Uniaxial tests at room temperature and DSC tests are carried out to iden-  
334 tify Cu-SC-SMA material parameters for the micromechanical behavior model  
335 ([Merzouki et al., 2010](#); [Collard and Ben Zineb, 2012](#)). Then, Cu-SC-SMA wires

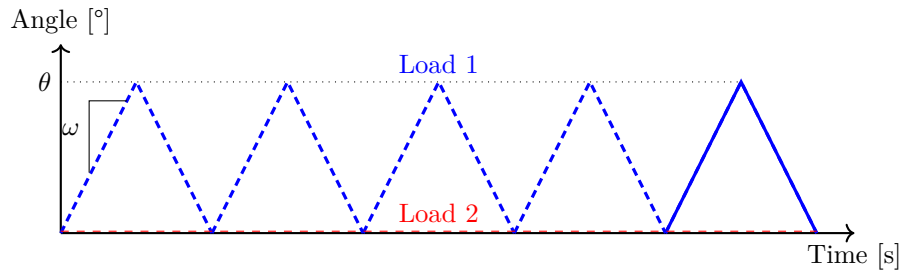


(a) Principle scheme of the testing device

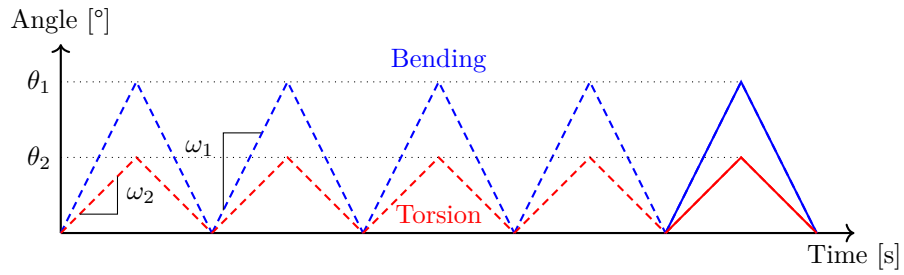


(b) Detailed picture of the testing device

Figure 5: Presentation of the testing device.



(a) Loading path for simple bending or torsion. Load 1 is equated with bending with an angle  $\theta$  of  $60^\circ$  and a rotation speed  $\omega$  of  $3^\circ.s^{-1}$  for a simple load of bending. It is equated with torsion with an angle  $\theta$  of  $30^\circ$  and a rotation speed  $\omega$  of  $1.5^\circ.s^{-1}$  for a simple load of torsion. Load 2 is the complementary load, set as  $0^\circ$ .



(b) Loading path for combined bending-torsion. Bending load is applied with an angle  $\theta_1$  of  $60^\circ$  and a rotation speed  $\omega_1$  of  $3^\circ.s^{-1}$ . Torsion load is applied with an angle  $\theta_2$  of  $30^\circ$  and a rotation speed  $\omega_2$  of  $1.5^\circ.s^{-1}$ .

Figure 6: Schematic description of the applied loads on endodontic files.

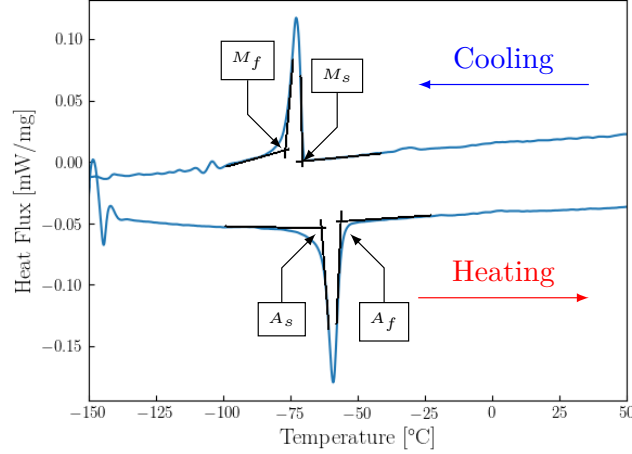


Figure 7: DSC results for a Cu-SC-SMA wire between +50°C and -150°C.

336 are experimentally and numerically tested in bending, torsion and combined  
 337 bending-torsion. The numerical responses issued from the micromechanical  
 338 model are compared to the experimental ones in order to check the ability  
 339 for the model to correctly predict wire tension response.

340 Figure 7 shows results of DSC tests on Cu-SC-SMA wire. They consist in  
 341 heating the sample up to 50°C then in cooling it down to -150°C twice and  
 342 in measuring the heat flux. The obtained results show two peaks, one while  
 343 cooling and one while heating, which are characteristic of forward and reverse  
 344 martensitic transformation respectively. The cooling peak is located between  
 345 -70°C and -78°C which determines  $M_s$  and  $M_f$ , the start and finish tempera-  
 346 tures for direct martensitic transformation, respectively. The heating peak is  
 347 visible between -63°C and -57°C which determines  $A_s$  and  $A_f$ , the start and  
 348 finish temperatures for reverse martensitic transformation, respectively. Figure  
 349 8 shows the uniaxial tension test for a Cu-SC-SMA wire of 0.79 mm diameter  
 350 subjected to 10 cycles of 8.5% strain. In addition, experimental tests of 30°  
 351 of bending, 5° of torsion and respectively 30° and 6° of combined bending and  
 352 torsion are realized on Cu-SC-SMA wires. Applied loadings are selected to show

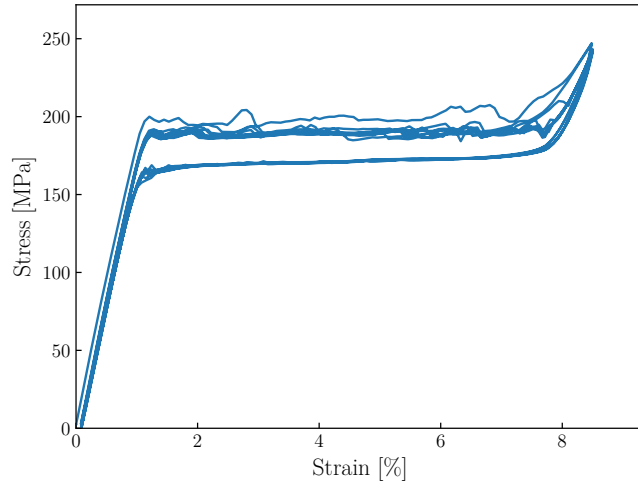


Figure 8: Uniaxial tension response of Cu-SC-SMA wire of 0.79 mm submitted to 10 cycles of 8.5% strain.

353 high deformation responses and not overpass range measurement of sensor. Fig-  
 354 ure 9 shows responses of these tests. Figure 9a gives the bending moment of a  
 355 Cu-SC-SMA wire subjected to bending and combined bending-torsion loading.  
 356 The elastic domain in both cases is similar until the activation of martensitic  
 357 transformation. Stiffness during transformation is more important in the case  
 358 of pure bending. Regarding the torsion moment of wire subjected to torsion  
 359 and combined bending-torsion loadings (figure 9b), responses to both loadings  
 360 show a high stiffness. Torsion loading on wire shows a linear response with very  
 361 low transformation. But, when torsion is combined with bending, the marten-  
 362 sitic transformation occurs in wire since the response of the material exhibits  
 363 a non linear behavior and a hysteresis between loading and unloading path.  
 364 Also, it is notable that the elastic domain of responses in pure and combined  
 365 bending-torsion has different stiffnesses.

366 In the following, the micromechanical model is used to represent the behavior  
 367 of Cu-SC-wire under tension, bending, torsion and combined bending-torsion  
 368 loadings.

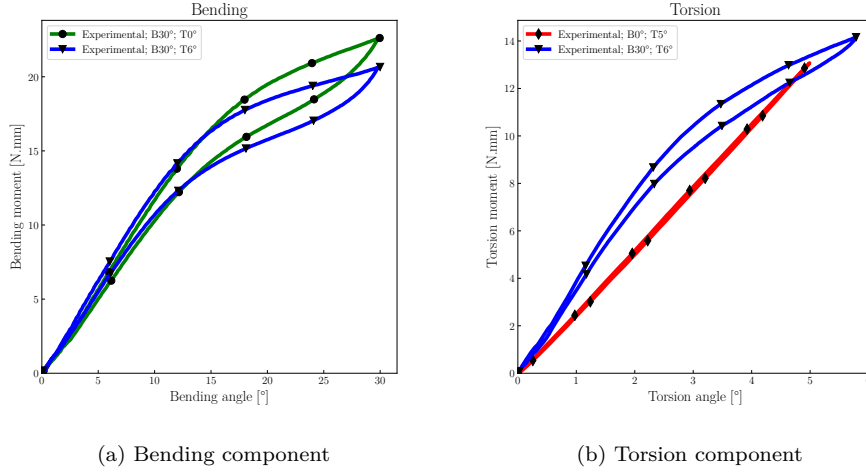


Figure 9: Cu-SC-SMA wire response under bending, torsion and combined bending-torsion loadings.

369 *3.3. Numerical and experimental comparison and material parameters identification*  
 370 *ation*

371 DSC tests, uniaxial tensile test, tests of bending, torsion and combined  
 372 bending-torsion are used to identify material parameters. DSC tests are used  
 373 to determine temperatures  $M_s$ ,  $M_f$ ,  $A_s$  and  $A_f$ . Elastic coefficients  $C_{11}$ ,  $C_{12}$   
 374 and  $C_{44}$  for austenite and martensite are identified from uniaxial tensile tests.  
 375 These tests also provide the maximum strain transformation.

376 According to the symmetric cubic elasticity approach (Belkahl, 1990), ma-  
 377 terial parameters presented in table 3 are used to identify the material parame-  
 378 ters the micromechanical constitutive law describing the behavior of Cu-SC-SMA.  
 379 Figure 10 compares the 10th cycle of uniaxial tension of figure 8 with the nu-  
 380 merical response of a unique cubic element submitted to 8.5% strain.

381 To complete material parameters identification, bending, torsion and com-  
 382 bined bending-torsion simulations are numerically predicted with previously  
 383 identified parameter. Numerical simulations are conducted with the boundary  
 384 conditions presented in section 2.2 to represent experimental loadings. Cu-SC-SMA

$C_{11}^A$ [MPa]	$C_{12}^A$ [MPa]	$C_{44}^A$ [MPa]	$A_f$ [°C]
123192	94200	110838	-57
$C_{11}^M$ [MPa]	$C_{12}^M$ [MPa]	$C_{44}^M$ [MPa]	$M_s$ [°C]
93456	94200	84084	-70
$\alpha$ [°C <sup>-1</sup> ]	B [MPa °C <sup>-1</sup> ]	C [MPa]	I [MPa]
1.5e-5	0.14	20-250	2500
g	$\phi_1$ [°]	$\Phi$ [°]	$\phi_2$ [°]
0.139	2	0	0

Table 3: Material parameters of Cu-SC-SMA wire used with micromechanical model

385 wires are represented with 27900 tetraedron elements with quadratic interpo-  
386 lation (codification: C3D10) in Abaqus<sup>®</sup> software. Figure 11 shows the compar-  
387 ison between experimental and numerical results for these loadings.

### 388 3.4. Comparison between numerical and experimental responses of Cu-SC-SMA 389 endodontic file prototypes

390 Endodontic file prototypes are manufactured from Cu-SC-SMA wire. They  
391 are tested under combined bending torsion loading with the testing device de-  
392 scribed in section 3.1. In addition, the numerical finite element model previously  
393 presented is used with a geometrical modeling of the blade of the endodontic  
394 file prototype. Both experimental and numerical responses are compared to es-  
395 timate the capacity of the model to represent a complex Cu-SC-SMA structure  
396 of endodontic file prototypes. The numerical model provides additional infor-  
397 mation compared to experiments such as stress state and martensitic variant  
398 volume fractions into the Cu-SC-SMA. Figure 12 shows the manufactured tested  
399 prototypes (figure 12a) and the corresponding finite element model (figure 12b).  
400 They have a two-edged cross section and their geometrical parameters are pre-  
401 sented in table 4. The finite element model is composed of 41600 tetrahedron  
402 elements with quadratic interpolation and represents only the blade of the pro-  
403 totype to reduce computing time. Three prototypes are tested in bending, torsion



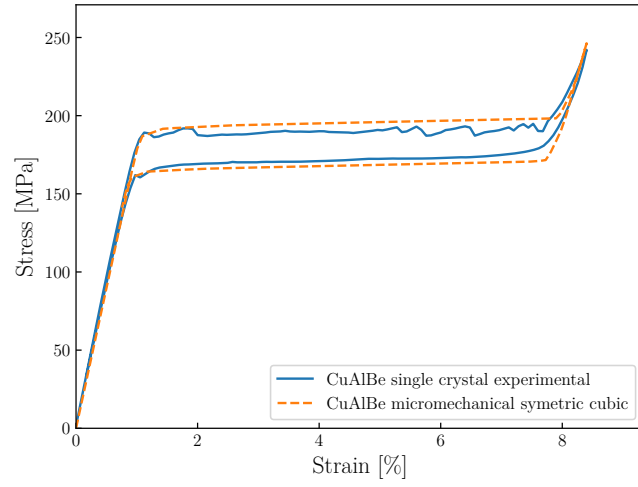


Figure 10: Experimental and numerical comparison of uniaxial tensile response of Cu-SC-SMA wire of 0.79 mm.

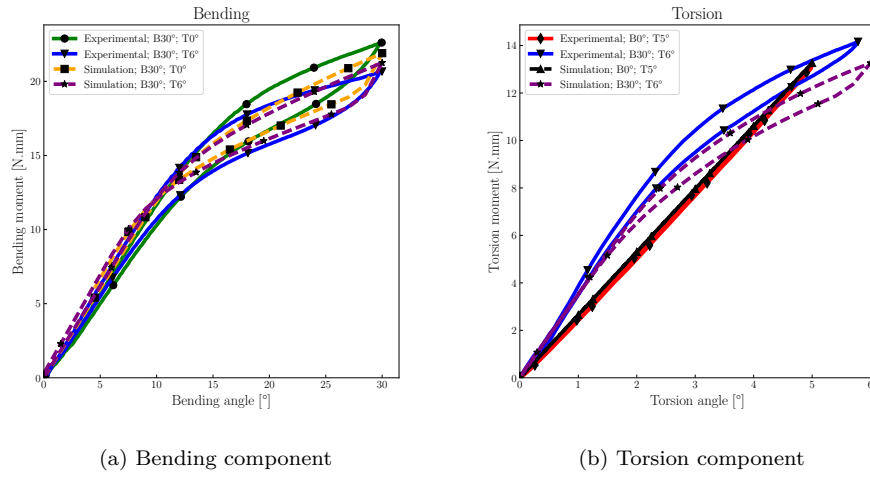
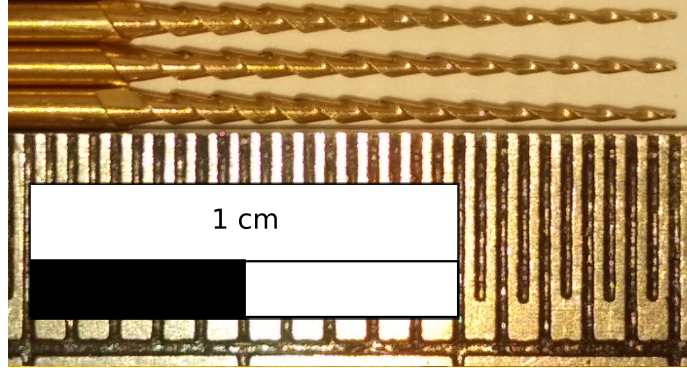
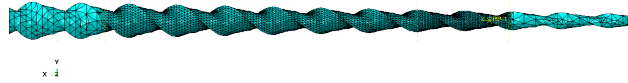


Figure 11: Experimental and numerical comparison of Cu-SC-SMA wire response under bending, torsion and combined bending-torsion loadings.




(a) Cu-SC-SMA endodontic file prototypes



(b) Modeled finite element of Cu-SC-SMA endodontic file prototypes

Figure 12: Single crystal endodontic file prototypes.

Table 4: Geometrical parameters of the tested prototypes.

Cross-section	Tip diameter	Taper	Pitch
	0.28 mm	4 %	1 mm

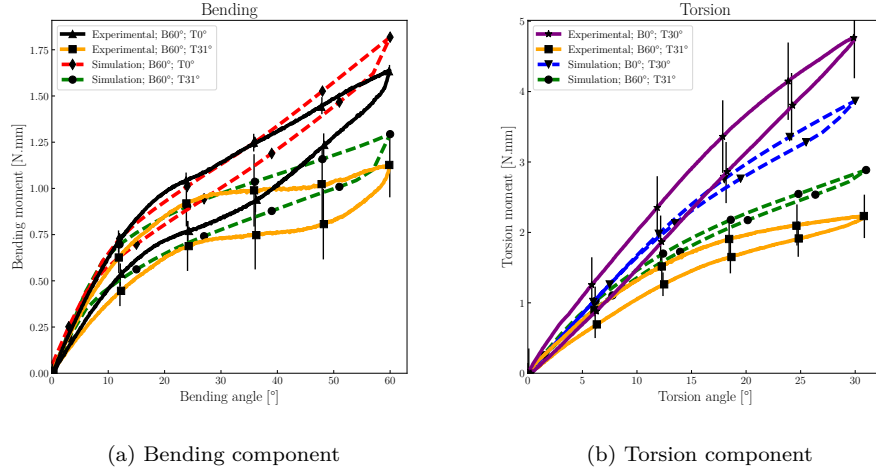


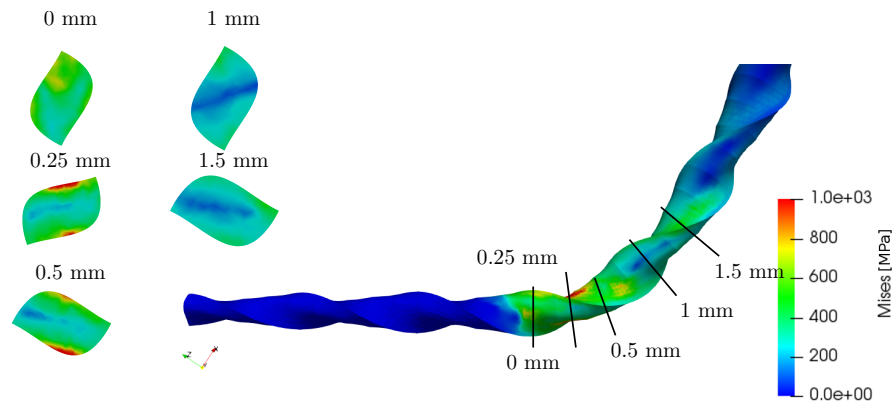
Figure 13: Compararion between experimental and numerical responses under bending, torsion and combined bending-torsion loadings of Cu-SC-SMA endodontic file prototypes with a tip diameter of 0.28 mm, 4% taper and two edges cross section.

404 and combined bending-torsion loadings. Their responses are averaged and the  
 405 standard deviation is displayed. The applied bending and torsion rotations are  
 406 respectively equal to 60° and 30°. Figure 13 presents experimental averaged  
 407 responses of prototypes under bending, torsion and combined bending-torsion  
 408 loadings. It is associated with numerical responses obtained with the finite  
 409 element model of equivalent geometrical endodontic file prototypes. It shows  
 410 that the numerical model predicts with a fairly good correlation the experimen-  
 411 tal response of the instrument. The effect of bending-torsion combination is  
 412 retranscribed by the model but some differences still exist. Martensitic trans-  
 413 formation starts earlier for the numerical model and the stiffness in torsion is  
 414 underestimated.

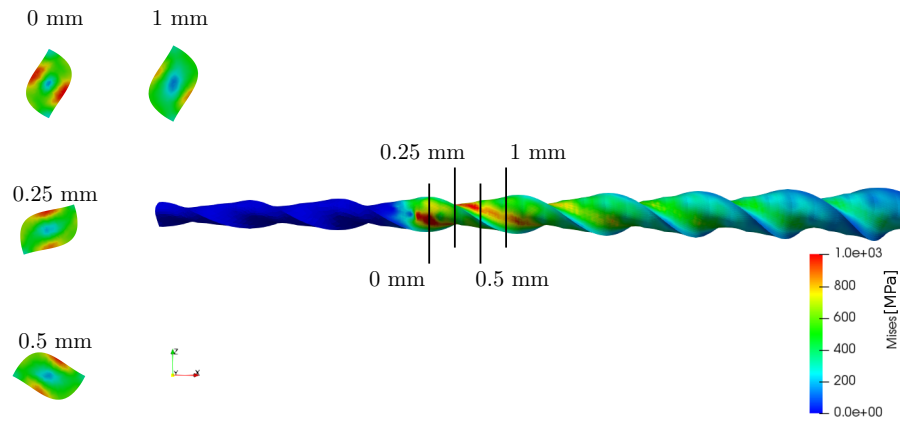
### 415 3.5. Stress and martensite volume fraction distributions

416 The presented finite element model allows to predict the local stress and  
 417 martenistic volume fraction in any material point of the instrument. Figures 14  
 418 and 15 depict the numerically obtained response for an endodontic file prototype

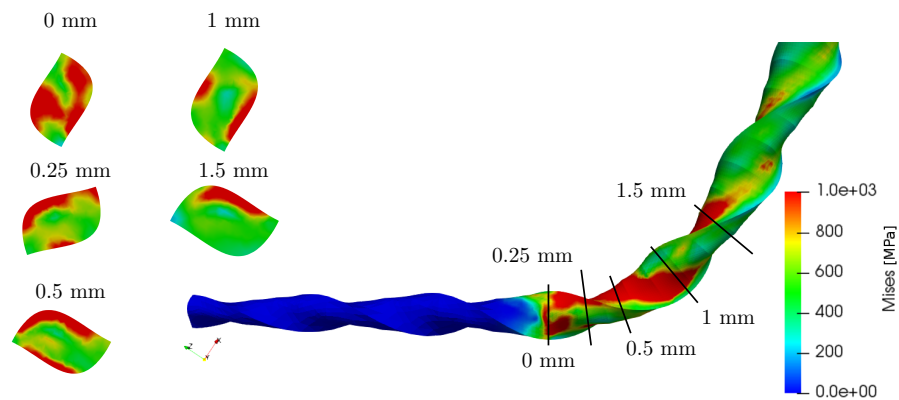
419 with a tip diameter of 0.28 mm, a 4% taper and a two-edged cross section, un-  
420 der bending, torsion and combined bending-torsion loadings. Bending loading  
421 induces a local stress concentration (figure 14a) in a zone close to the clamped  
422 area. Figure 15a shows that martensite appears in this zone subjected to ten-  
423 sion and compression. Figure 14b shows the results of torsion loading. A high  
424 stress state appears in all blade structures. It corresponds to a high stiffness of  
425 numerical and experimental responses. The stress distribution is mainly con-  
426 centrated in the center of the blade faces, close to the clamped area. Moreover,  
427 the numerical model predicts a low value of volume fraction of martensite (fig-  
428 ure 15b) for the Cu-SC-SMA endodontic file prototype in torsion. For combined  
429 bending-torsion loading (figure 14c), high stress levels concentrate in the bended  
430 zone of the instrument. The stress distribution is induced by a superposition  
431 of the stresses obtained by bending and by torsion with the addition of the  
432 complex geometry effect. Figure 15c shows the volume fraction of martensite  
433 for the combined bending-torsion loadings. It follows the stress distribution,  
434 visible for the 0 mm, 0.25 mm, 0.5 mm cuts. However, 1 mm and 1.5 mm cuts  
435 show differences in the distribution of stress and volume fraction of martensite.  
436 For the 1 mm cut, on figure 15c, volume fraction of martensite is concentrated  
437 in inner and outer part of the bended area when the stress distribution (figure  
438 14c) corresponds to torsion loading. Moreover, the numerical model allows to  
439 determine the activated martensite variants and their associated volume frac-  
440 tion in each material point. Figure 16 gives, for the main active variants, the  
441 zone where each variant occurs with its associated volume fraction. These vari-  
442 ants are 7, 13, 14 and 22 defined in table 1. Their distributions show that each  
443 martensite variant occurs separately and partially cohabits with other variants  
444 depending on their compatibilities (table 2). Variant 14 occurs in the inner side  
445 of the bended area (subjected to a compression stress) next to variants 7 and  
446 22. According to table 2, variants 7-22 are incompatible, but 7-14 and 14-22 are  
447 compatible. Variant 13 occurs especially in the outer side of the bended area.  
448 Moreover, variants in tension and compression areas are different. Variants 13



(a) Bending

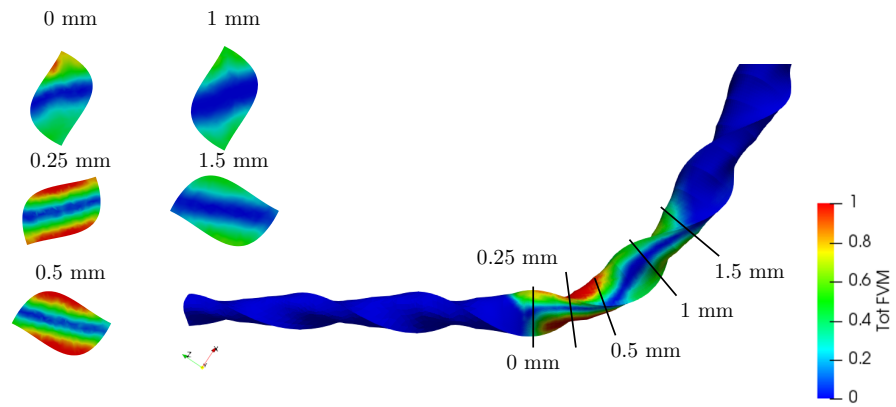


(b) Torsion

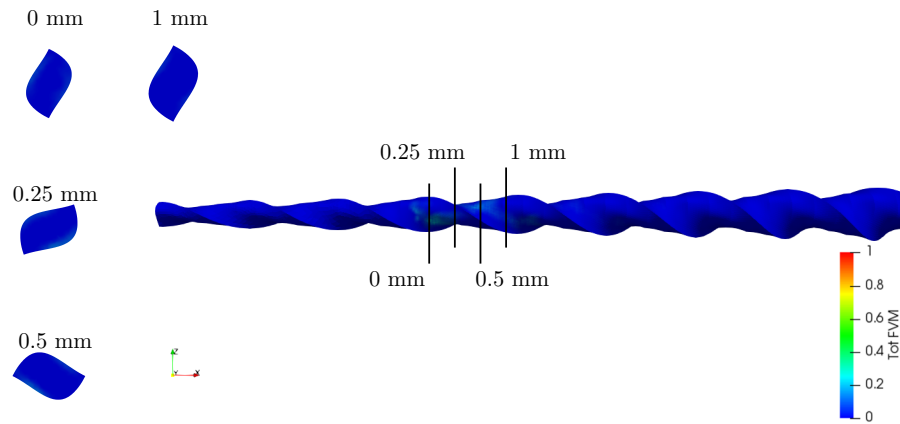


(c) Combined bending-torsion

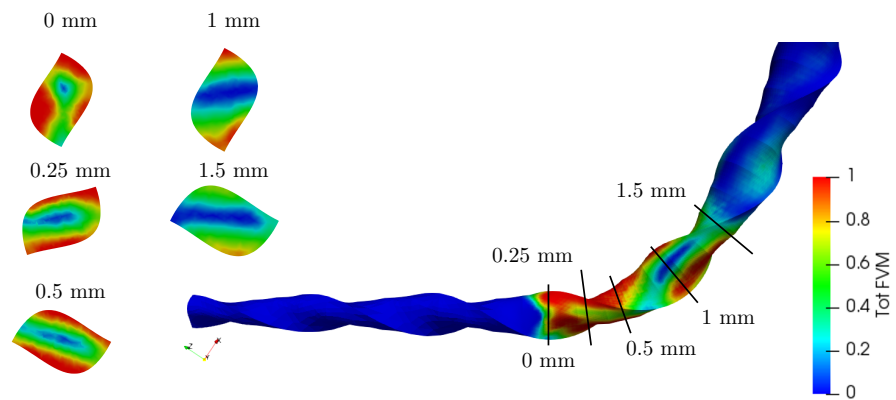
Figure 14: Stress distribution in an endodontic file prototype with a tip diameter of 0.28 mm, a taper of 4% and two edges cross section made of Cu-SC-SMA submitted to bending, torsion and combined bending-torsion loadings. Clamped area is 3 mm length.



(a) Bending



(b) Torsion



(c) Combines bending-torsion

Figure 15: Volume fraction of martensite distribution in an endodontic file prototype with a tip diameter of 0.28 mm, a taper of 4% and two edges cross section made of Cu-SC-SMA submitted to bending, torsion and combined bending-torsion loadings. Clamped area is 3 mm length.

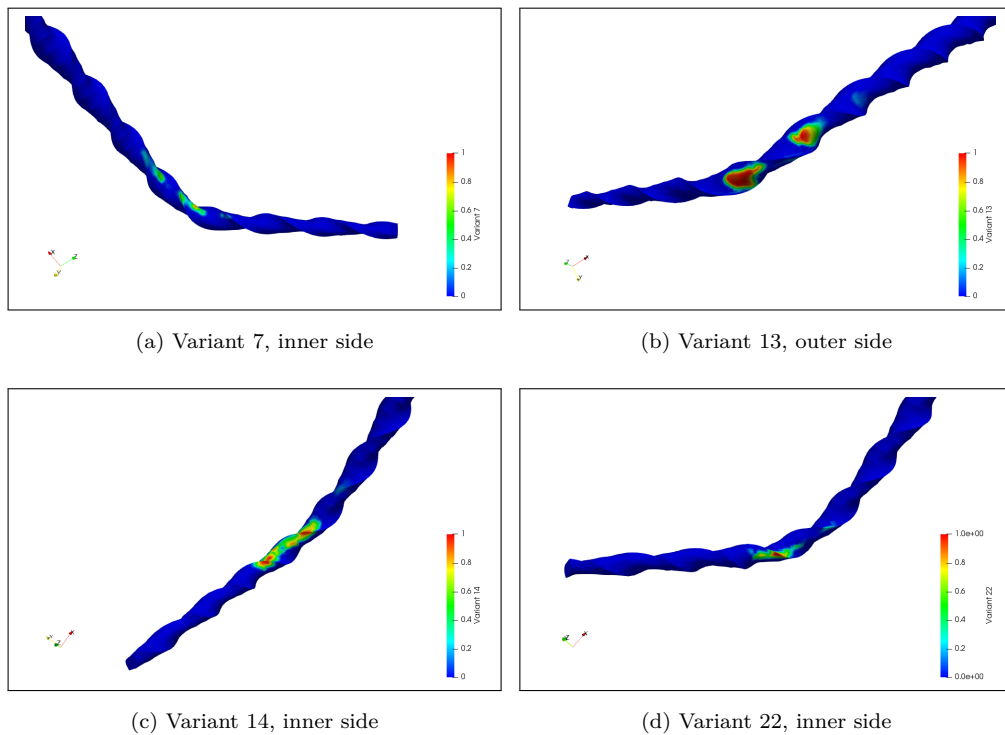





Figure 16: Distribution of variants 7, 13, 14 and 22 in combined bending-torsion loading. Their transformation direction and normal plane are given in table 1 and their interactions in table 2.

Table 5: Selected factors with their corresponding levels used in the Taguchi design of experiment.

Factor	Level 1	Level 2	Level 3
Cross Section	 0.5pt Asymmetric		
Tip diameter at 3 mm	0.40 mm	0.45 mm	0.50 mm
Taper	3 %	4 %	5 %
Pitch length	0.70 mm	0.85 mm	1.00 mm

449 and 14 are compatible but they occur for different loading levels in the bended  
 450 area.

451 **4. Influence of the geometrical parameters on the response of the**  
 452 **studied endodontic files**

453 After the identification of material parameters for the Cu-SC-SMA used  
 454 to manufacture endodontic file prototypes, a Taguchi design of experiment is  
 455 carried out numerically. It enables to analyse the influence of the geometrical  
 456 parameters on the global response of these endodontic files during combined  
 457 bending-torsion loading. It is designed to study multiple factors with a minimum  
 458 number of simulations on the system and reduces the computation time.

459 *4.1. Selected factors and levels*

460 For this study, the selected factors are the cross section shape, the tip diam-  
 461 eter at 3 mm from the tip, the taper and the pitch of the blade. Each factor  
 462 has 3 levels represented in table 5.



Table 6: Taguchi orthogonal table with 4 factors at 3 levels.

Test	Factor 1 (Cross Section)	Factor 2 (Tip diameter at 3 mm)	Factor 3 (Taper)	Factor 4 (Pitch)
1	1	1	1	1
2	1	2	2	2
3	1	3	3	3
4	2	1	2	3
5	2	2	3	1
6	2	3	1	2
7	3	1	3	2
8	3	2	1	3
9	3	3	2	1

463 *4.2. Orthogonal table selection*

464 The selected set of factors and their levels are suitable for a Taguchi orthog-  
465 onal table  $L9(3^4)$  presented in table 6. Each factor is assigned to a column  
466 where its values vary between the previously selected levels. Each line repre-  
467 sents a numerical simulation to perform on the system with the levels of the  
468 corresponding factor in columns. According to this table, it is possible to model  
469 the corresponding blade geometries, which are presented in table 7.














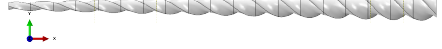




470 *4.3. Equivalent combined bending-torsion response*

471 The modeled endodontic file prototype responses are then numerically ana-  
472 lyzed in combined bending-torsion. The adopted equivalent moment response  
473 of combined bending-torsion  $M_{eq}$  is defined by the following relation:

$$M_{eq} = \sqrt{M_{bending}^2 + 3 \times M_{torsion}^2} \quad (11)$$

474 where  $M_{bending}$  and  $M_{torsion}$  are the moment responses of simulated prototypes  
475 for bending and torsion respectively. Numerically obtained results are post-

Table 7: Selected factors with their corresponding level used in the Taguchi design of experiment according to table 6.

Prot.	Cross Section	$\varnothing_{at\ 3mm}$	Taper	Pitch	Modeled prototype
N#	[-]	[mm]	[%]	[mm]	
1		0.40	3	0.70	
2		0.45	4	0.85	
3		0.50	5	1.00	
4		0.40	4	1.00	
5		0.45	5	0.70	
6		0.50	3	0.85	
7		0.40	5	0.85	
8		0.45	3	1.00	
9		0.50	4	0.70	

476 treated to express the variation of the equivalent moment response around the  
477 mean equivalent moment response of all tests.

#### 478 *4.4. Numerical results issued from the Taguchi DOE*

479 Simulated responses of combined bending-torsion loadings for endodontic file  
480 prototypes in Cu-SC-SMA are depicted in figure 17. Figure 18 is the graphical  
481 representation of the mean response of the finite element model for a given factor  
482 level. It consists in making the average of all the responses for the observed  
483 factor level. Since the Taguchi table is orthogonal, the influence of other factor  
484 levels is equivalent for each observed factor level.

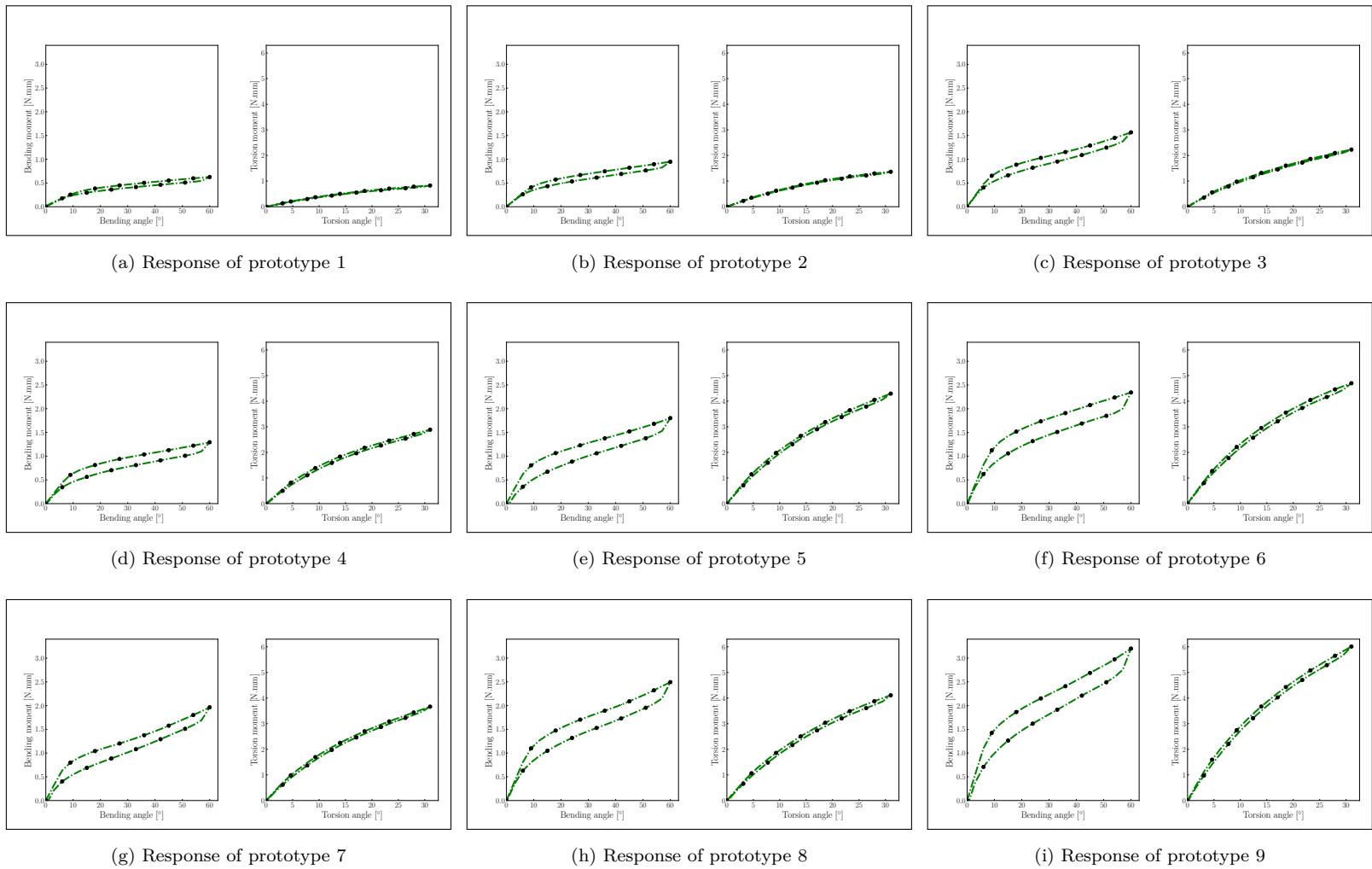


Figure 17: Responses in bending and torsion of the 9 finite element model prototypes.

485 According to the mean numerical responses of the factor levels, the best  
486 parameters to reduce the global moment response in combined bending torsion  
487 loading are: the asymmetric section shape, a diameter at 3 mm from the tip of  
488 0.40 mm, a taper of 4% and a 1 mm pitch length. The evolution of the diameter  
489 at 3 mm from the tip and the pitch length shows linear global response variation  
490 while the taper seems to minimize this response for a value of 4%. The parameter  
491 inducing the widest variation in the response is the cross section, followed by  
492 the diameter at 3 mm from the tip , the taper and finally the pitch length.

493 .

494

## 495 5. Discussions

### 496 5.1. Introduction

497 In this section, experimental and numerical results are detailed and dis-  
498 cussed. The first part presents experimental data of uniaxial tension, bending,  
499 torsion and combined bending-torsion tests on Cu-SC-SMA wires and endodon-  
500 tic file prototypes with their numerical comparison. The second part presents  
501 the analysis of the results of the Taguchi DOE. The third part analyzes distri-  
502 butions of stress and of martensitic variants in endodontic file prototypes loaded  
503 in bending, torsion and combined bending-torsion.

### 504 5.2. *Experimental and numerical comparison of bending, torsion and combined* 505 *bending-torsion responses with Cu-SC-SMA endodontic file prototypes*

506 The comparison between the experimental and numerical responses in bend-  
507 ing, torsion and combined bending-torsion loadings depicted in figures 11 for  
508 wire and 13 for endodontic file prototype in Cu-SC-SMA, shows satisfactory  
509 correlations. The material parameters, identified from DSC measurements, ten-  
510 sion and torsion tests, allow to predict the Cu-SC-SMA response under tension  
511 and torsion loadings as shown on figures 10 and 11b. Numerical prediction in  
512 bending and combined bending-torsion tests on Cu-SC-SMA wires are slightly

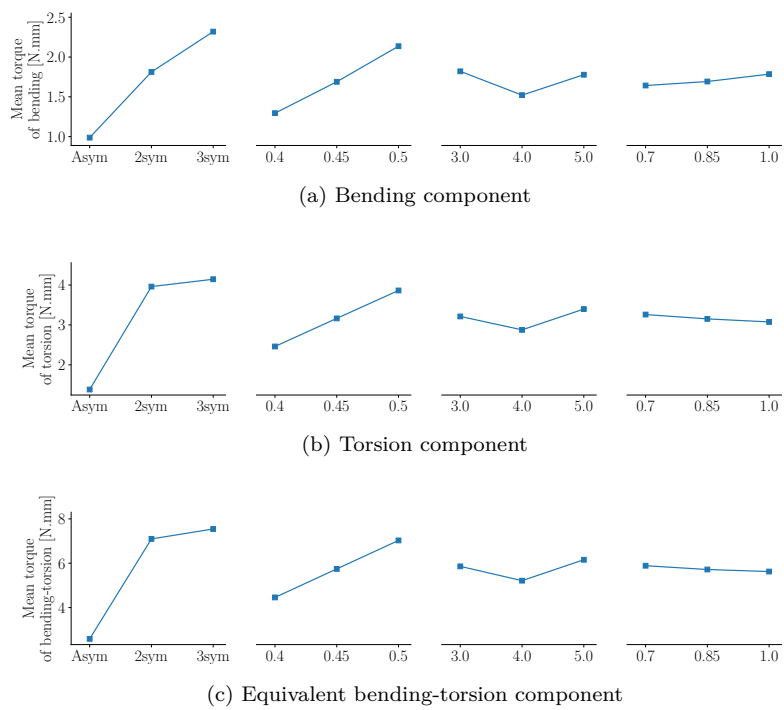


Figure 18: Mean responses according to level factor of endodontic file prototype in Cu-SC-SMA under combined bending-torsion.

513 less correlated with the experimental responses (figure 13). However, numerical  
514 and experimental tendencies, such as the decrease of the transformation plateau  
515 stiffness, observed between bending and combined bending-torsion is satisfacto-  
516 rily predicted by the numerical model (figure 11a). In addition, elastic stiffness  
517 increases and appearance of hysteresis in torsion component for numerical re-  
518 sponse in combined bending-torsion loading (figure 11b) is well predicted by the  
519 model. However, the numerical torsion response in combined bending-torsion  
520 loading is under rated compared to experimental results.

521 The results issued from experimental and numerical predictions of the en-  
522 dodontic instrument response under bending, torsion and combined bending-  
523 torsion loadings are in satisfactory agreement. The differences between the two  
524 results need to be solved with enhancement of the adopted finite element model.  
525 On the one hand, elastic stiffness in torsion loading is underestimated (figure  
526 13b). Likewise, in bending loading, the martensitic transformation predicted by  
527 the numerical model shows a smaller hysteresis than the experimental response.

528 Several sources can explain these differences. On the experimental side, the  
529 machining process with its imprecision may have an impact on the anticipated  
530 shape of the prototypes. Likewise, the clamp of the tip, may generate addi-  
531 tional stresses in the area close to the bended one. Moreover, high loading  
532 amplitudes are severe to the prototype instrument, which is brought to its me-  
533 chanical limits and over the clinically acceptable work condition. Furthermore,  
534 these loading conditions may generate plasticity, which is not taken into ac-  
535 count by the adopted thermomechanical constitutive model, and could explain  
536 the difference in martensitic transformation between experimentally measured  
537 and numerically predicted responses. The aforementioned causes also have an  
538 impact on the modeling part. Indeed, the modeled prototype is assumed perfect,  
539 without any machining imprecisions or microstrural change, like local recrystal-  
540 lization. In addition, the model represents idealized clamping conditions of  
541 contact between a plane and the tapered helicoidal triangular section shape.

542 On the other hand and despite all these difficulties, the micromechanical  
543 model is able to closely reproduce the response of Cu-SC-SMA endontic file

544 prototypes under separated and combined bending-torsion loadings. The com-  
545 parison of the bending component of the global numerical response between  
546 bending and combined bending-torsion (figure 13a) shows that the model cor-  
547 rectly predicts the decrease of the response after the start of martensitic tran-  
548 sformation. For the torsion component, the decrease observed between combined  
549 and separated torsion responses, on figure 13b, shows the model capacities to  
550 reproduce global behavior of Cu-SC-SMA for complex loading cases.

### 551 *5.3. Distribution of stresses and volume fraction of martensite through the en-* 552 *doodontic file*

553 Figures 14 and 15 depict the stress and volume fraction of martensite in  
554 endodontic file prototypes made of Cu-SC-SMA. It is visible that bending and  
555 torsion loadings, in figures 14a and 14b respectively, generate high stress lev-  
556 els, but only bending loading activates martensitic transformation (figure 15a).  
557 Despite a high shear stress, concentrated in the middle of the blade faces of  
558 the Cu-SC-SMA prototypes in torsion loading, a low quantity of martensite  
559 is produced (figure 15b). Figure 14c shows how bending and torsion loadings  
560 interact in combination and their influence on the martensitic transformation  
561 level and its location (figure 15c). The Von Mises equivalent stress distribu-  
562 tion for combined bending-torsion is a superposition of both normal and shear  
563 stress distribution. The volume fraction of martensite is diffused according to  
564 this stress distribution, except for stresses present in the middle of blade faces,  
565 close to the 1 mm cut from the clamped area, and beyond (figure 15c). In the  
566 case of combined bending-torsion loading, torsion increases the stiffness of the  
567 instrument, leading to a more important martensitic transformation induced  
568 by bending. Moreover, the complex geometry of the instrument leads to more  
569 complex three-dimensional stress state. This directly influences the activation  
570 process of martensitic variants (figure 11b and 13b). In addition, the flexibil-  
571 ity gain in torsion of numerical responses between pure torsion and combined  
572 bending-torsion loadings is visible with the transformation plateau on figure



573 **13b.** It is a global effect due to the martensitic transformation initiated by  
574 bending.

575 Moreover, from the combined bending-torsion loading, the activated marten-  
576 site variants are different for those activated for separated bending and torsion  
577 loading. It induces a higher quantity of martensite and thus a higher transfor-  
578 mation strain. Therefore, the induced global stiffness in torsion is lower for the  
579 combined bending-torsion than in pure torsion. In addition, combining bending  
580 and torsion leads to a higher failure level in torsion rotation than in the case of  
581 pure torsion.

#### 582 *5.4. Accurate geometry according to Taguchi DOE*

583 The Taguchi DOE allows to choose the best set of geometrical parameters,  
584 for the response prediction of endodontic file prototypes in Cu-SC-SMA under  
585 combined bending-torsion loading. This parameter set leads to the lowest stiff-  
586 ness in combined bending-torsion. According to figure 18, it corresponds to an  
587 asymmetric cross-section, with diameter at 3 mm from the tip of 0.4 mm, a  
588 taper of 4% taper and 1 mm pitch length. The most influent parameter is the  
589 cross-section. The asymmetrical part of the cross section offers the best op-  
590 tion acting on the moment-rotation global responses. The taper has the lowest  
591 influence on the moment-rotation global response. These results are obtained  
592 with the numerical analysis and shown in figure 17. Moreover, during canal  
593 root preparation, the diameter and the taper of the endodontic file are chosen  
594 according to the size of the tooth canal. To go further, experimental investi-  
595 gations should lead to a better prediction of the influence of each geometrical  
596 parameter for endodontic files. Numerical simulations consider ideal geometry.  
597 They should be replaced by the exact geometry of the manufactured endodontic  
598 files with their imperfection.

## 599 **6. Conclusion and prospects**

600 This paper details the experimental and numerical response of a Cu-SC-SMA  
601 endodontic file subjected to a bending-torsion loading. This new endodontic

602 instrument makes the preparation of root canal with higher simple or double  
603 curvature easier. In addition it has very interesting antimicrobial properties. A  
604 specific bending-torsion testing device is designed and manufactured in order  
605 to carry out the experimental analysis. The corresponding obtained results  
606 enable to identify the material parameters of a micromechanical constitutive  
607 law, well adapted to Cu-SC-SMA. This law is coupled with a finite element  
608 method to simulate the response of the studied endodontic file prototypes under  
609 several loadings. It depicts an increase in the torsion strength of these Cu-SC-  
610 SMA endodontic files when subjected to a combined bending-torsion loading  
611 in comparison with a response for a pure torsion loading. The parameterized  
612 geometrical model enables to analyze the influence of geometrical parameters  
613 on the global response of these endodontic files. A Taguchi experimental plan is  
614 applied for this analysis. It shows that the best parameter settings to decrease  
615 moments in combined bending-torsion loading is an asymmetric section shape,  
616 the lowest diameter at 3 mm from the tip of 0.4 mm, a taper of 4% and a pitch  
617 length of 1 mm.

618 In conclusion, the obtained numerical and experimental results show that  
619 the different responses of the instruments made of Cu-SC-SMA are close to  
620 what was observed for commercial NiTi based instruments ([Schäfer and Tepel, 2001](#);  
621 [Ninan and Berzins, 2013](#); [Santos et al., 2016](#)) and the sensitivity to geo-  
622 metrical parameters is also globally the same. It should be possible to consider  
623 endodontic files made of Cu-SC-SMA to maximize micro-organisms elimina-  
624 tion while shaping the root canal, and to reduce the risks of failure during  
625 endodontic treatment. The main challenges will be the optimization of their  
626 shaping performances during the root canal preparation and the carrying out  
627 of clinical tests in order to validate such performances in-vivo. Moreover, the  
628 manufacturing process of the instrument could modify the Cu-SC-SMA behav-  
629 ior. Additional features should be implemented in the micromechanical model  
630 to fully exploit its potential to study microstructure of endodontic files under  
631 rigorous constraints, such as plasticity or clamped conditions on the tip which  
632 can be improved. Finally, future investigations should explore the shape mem-

633 ory effect of Cu-SC-SMA to investigate the possibilities of an increase of the  
634 transformation capacities in torsion of this SMA, which can be favorable in the  
635 endodontic domain.

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