Experimental and numerical investigations of cutting forces and chip formation during micro-cutting of Ti42Nb titanium alloy produced by laser-based powder bed fusion

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Abstract

Ti-Nb alloys are high-profile candidates for the biomedical applications. However, because of poor surface integrity (i.e. residual stress and surface roughness), Ti-Nb implantable medical devices need to be machined in order to obtain functional surfaces finish. In this work, experimental and numerical investigations are conducted to study the micro-cutting response of Ti42Nb titanium alloy produced by laser-based powder bed fusion. Experimental micro-cutting tests are carried out using precision turning lathe. Trials are performed with two cutting velocities of 60 m/min and 120 m/min and different feed rates, varying from 5 to 40 $\mu$m/rev. For the numerical study, a porous crystal plasticity-based model is proposed to address the impact of anisotropy and microstructure heterogeneities of the polycrystalline material. The crystal plasticity-based model is identified using strain–stress curves obtained from compression
tests performed under two strain rates and a wide range of temperatures. Numerical micro-cutting simulations are performed in order to gain insight into the impact of microstructural features (i.e. crystallographic orientation and grain size) on the machinability of the alloy. According to the results, the effect of the strain rates and the temperature on the thermomechanical behavior of the Ti42Nb titanium alloy produced by laser-based powder bed fusion is correctly depicted. The model captured the strain localization on adiabatic shear band during compression tests. According to the micro-cutting simulations, the local variables such as temperature, damage and plastic deformation are strongly impacted by the crystallographic orientations and the grain size. In addition, depending on the crystallographic orientations, the chip morphology changes form continues, slightly segmented to largely segmented.

**Keywords:** Micro-cutting, Thermodynamics, Crystal plasticity, Finite strain, Continuum damage model, Ti42Nb titanium alloy

1 Introduction

The impact of the microstructure on the cutting forces and the chip formation process is a complex subject to address during cutting operations [27, 35, 2, 14]. On the first hand, it is quite difficult to vary independently the microstructural features (e.g. grain size, crystallographic texture, phases) [36, 16, 34]. On the other hand, during cutting operation, the microstructure is subjected to severe loading conditions (high temperature, high strain rates and large deformations) which lead to microstructure transformations mainly in the chip formation zone. It is therefore not possible to keep constant the microstructure during the cutting operations. As a result, it is necessary to understand the role of the initial microstructure and the microstructure transformations and their effects on the behaviour of the material in the cutting zone.

Some studies have shown the strong dependence of titanium alloys machinability to the initial microstructure. Indeed, the investigations conducted by Ramirez [26] highlighted the impact of the morphological texture of both α and β phases on the chip formation for heat treated α + β TA6V titanium alloy. In the above study, two microstructures have been tested: (i) a bimodal α + β microstructure composed of primary α grains in a β matrix and (ii) a lamellar microstructure consisting of α lamellae embedded in a β matrix. The chip obtained during the cutting operations of the bimodal microstructure is slightly segmented while the chip segmentation is much more pronounced for the lamellar microstructure. Relationships between the morphological orientation of the α lamellae and the localization of the plastic deformation were proposed by Barelli [4] in orthogonal milling and Wagner et al [32] in turning for the heat-treated α + β TA6V titanium alloy. The effect of the fraction of β phase on the TA6V chip formation was investigated by Joshi et al [15].
In order to better understand the mechanisms of chip formation during cutting operations, different experimental techniques have been used to obtain kinematic data (i.e. displacement field), thermal or mechanical data (i.e. temperature and cutting forces fields) \cite{25, 24, 8}. These techniques allow an access to the temperature and deformation fields, which are essential to obtain the thermo-mechanical loads that undergo the tool and the workpiece. In the recent years, experimental studies have been made to establish a thermo-mechanical balance of the chip formation process from simultaneous thermal and kinematics measurements \cite{25, 12}. Despite, these measurements have been successfully applied for uniaxial tests (i.e. tensile, shear...), the development of a simultaneous measurement of strains, strain rates and temperatures at the tool chip interface to understand the chip formation genesis is extremely difficult and few studies have been carried out in the case of cutting \cite{37, 13}. If the measurements allow to build large experimental databases, some informations remain inaccessible. Thus, experimental technique does not allow to obtain the stress field during the cutting operation. Moreover, the experimental techniques listed above provide only partial informations, notably because that the measurements are obtained on the lateral surfaces of the workpiece and the formed chip.

It is possible to overcome these difficulties by using the numerical simulations of chip formation \cite{1, 20}. On the one hand, a primary interest of the numerical simulations is the ability to access the thermal, kinematic and mechanical fields \cite{9, 28}. On the other hand, the numerical simulations allow to study the impact of material properties on tool/chip interaction \cite{6, 7}. During cutting of metallic materials specificity those obtained through additive manufacturing technologies, the size of the microstructural heterogeneities can be comparable to the cutting volume. The cutting operations occur therefore inside single grain. By consequence, the material behavior can not be considered as homogeneous and isotropic. It is therefore necessary to consider the impact of local microstructure (e.g. orientation of the individual grains, phases) on the surface integrity and machining response.

In order to incorporate the impact of microstructure heterogeneities (i.e. the different phases of AISI 1045 steel), Simoneau et al. \cite{29, 31, 30} have developed cutting simulations with two material phases modelled using Johnson-Cook behavior law with different coefficients to account for the hard phase. This work highlighted the impact of the material heterogeneities on the morphology of the formed chip. An explicit modelling of titanium microstructures was used in cutting simulations by Zhang et al. \cite{38}. The grains were explicitly modelled and randomly oriented. A 2D model with plane deformations hypothesis was adopted. A crystal plasticity based model was applied to describe the individual behavior of the HCP $\alpha$ and the BCC $\beta$ phases. Ayed et al. \cite{3} extended the above approach by suggesting a 3D modelling of the grains by Voronoi cells. According to the authors, a notable change in the $\beta$-grains orientations was observed during cutting process. Recently, Wang et al. \cite{33} have developed a crystal plasticity based model for diamond tool
cutting polycrystalline copper. The cutting model has the advantage of taking into account large deformations. The cutting simulations are performed in 2D. The grains were explicitly modelled and the crystallographic orientations were obtained from EBSD analyses. A crystal plasticity constitutive law was applied to model the individual crystal behavior. According to the results, cutting forces showed a high dependence to the local texture. Cutting simulations illustrated a heterogeneous plastic deformation in the formed chip zone.

Despite the acceleration of the use of titanium alloy on the manufacturing of medical devices through the additive manufacturing technologies, parts produced in-situ by laser-based powder bed fusion show poor surface quality and need to be machined in order to obtain functional surface. The as-LB-PBFed Ti42Nb alloy shows also an anisotropic mechanical behavior and a heterogeneous microstructure that lead to complex thermo-mechanical response. Therefore, understanding the impact of microstructural features during microcutting under extreme loading conditions is of great industrial interest that will further leads to optimize the machining conditions, to reduce the cost and to increase the productivity. In this work, experimental and numerical analyses have been performed in order to study the micro-cutting response of Ti42Nb titanium alloy produced by laser-based powder bed fusion. Experimental investigations have been carried out using precision turning lathe. Numerical simulations have been performed to address the impact of crystallographic orientation and grain size of the single $\beta$-phase polycrystalline material during micro-cutting. This paper is organized as follows. In the first section, the experimental equipment and methodology are described. In the second section, the constitutive relations using the framework of continuum thermodynamics is detailed. Then, the identification procedure of the model parameters is presented. Finally, orthogonal micro-cutting simulations are performed and compared to the experimental findings.

## 2 Experimental equipment and methodology

### 2.1 Material

In this study, Ti42Nb alloy is manufactured from the elemental mixture of spherical Ti and Nb powders. The particle size distributions, which are measured by laser diffraction, reveal that Ti particles sizes ranged from $D_{10} = 26 \mu m$ to $D_{90} = 118 \mu m$ with $D_{50} = 62 \mu m$ while the size of Nb particles is $D_{10} = 12 \mu m$, $D_{50} = 44 \mu m$ and $D_{90} = 90\mu m$. The chemical composition of the Ti42Nb titanium alloy investigated in this work is presented in Table 1.

<table>
<thead>
<tr>
<th>Element</th>
<th>Ti</th>
<th>Nb</th>
<th>C</th>
<th>S</th>
<th>H</th>
<th>N</th>
<th>O</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mixed powder</td>
<td>57.29</td>
<td>42.5</td>
<td>0.029</td>
<td>0.007</td>
<td>0.005</td>
<td>0.007</td>
<td>0.18</td>
</tr>
</tbody>
</table>
The LB-PBF parameters such as laser power, scanning speed, scanning spacing and layer thickness are described in a previous communication [5]. In order to investigate the possible impact of anisotropy, two building directions are used for manufacturing the compression and micro-cutting specimens. A first batch is produced with a building direction parallel to the Z-axes of the LB-PBF machine. Then, a building direction rotated by 45° with respect to the Z-axes is selected for manufacturing the second batch of specimens. Compression and micro-cutting tests are performed on specimens elaborated using the two building directions.

Fig. 1 (a) Scanning electron microscopy (SEM) observations showing the as-LB-PBFed Ti42Nb microstructure of specimen produced with a building directions of 90°, the undisolved Nb particles and the pores (b) Electron Backscatter Diffraction (EBSD) map taken in the center of the specimen.

Figure 1-a shows the scanning electron microscopy (SEM) observations of the Ti42Nb microstructure. According to the results, the Ti42Nb microstructure is composed of non-columnar elongated β-grains oriented along the building direction. The as-LB-PBFed Ti42Nb microstructure shows the presence of un-melted or partially melted Nb particles (tomography analyses prove that the un-melted Nb particles represent less than 1% of the total amount of the Nb mass in the alloy see [5]) and spherical and elliptical pores distributed over all the specimens. These pores do not have preferential nucleation sites. Electron backscatter diffraction (EBSD) analyses highlighted the existence of preferred crystallographic orientation (see Figure 1-b). According to the results, a crystallographic orientation \(\{001\} \langle 100 \rangle\) is observed. Also, according to these observations, the average grain size is about 80 µm.
2.2 Experimental equipments

The compression tests are conducted under two strain rates (1 s\(^{-1}\) and 10 s\(^{-1}\)) and different temperatures (298 K, 673 K, 873 K and 1073 K) using a Gleeble 3500 machine. For these tests, cylindrical specimens (with a diameter 6 mm and 9 mm in height) are manufactured by laser-based powder bed fusion. The elongation and the temperature are measured using an axial extensometer and a K-type thermocouple. Compression tests are performed with a constant nominal strain rate up to the fracture of the specimens. Finally, the specimens are cooled rapidly to room temperature using a compressed-air jet. Micro-cutting trials for this study is carried on a 5 axis ROEDERS RXP200DS, with a maximum spindle speed of 60 000 rpm. The CNC vertical milling is used as an accurate precision turning lathe by positioning a cylindrical sample on the spindle, see figure 2. The micro-cutting cylindrical specimens are first prepared to obtain a 6 mm diameter, with an acceptable roughness, to be clamped on a precision tool holder BIG Mega HSK E25 defined as tube holder. The specimens are then internal and external turned by two roughing tools, to attain the desired tube width (\(w\)) (see figure 2). This method allows to get a limited workpiece run out and to verify the exact width by a TESA VISIO profilometer. The cutting tool selected is a micro turning tool IFANGER MTNY 41015-R with a nominal rake angle of 8° and a flank angle of 5°. The cutting-edge radius \(R_e\) was previously measured using an Alicona Infinite Focus 3D microscope and was close to 5 \(\mu\)m. Micro tool is mounted into a tool holder, fixed on a dynamometric table Kistler Minidyn 9256C2, associated with a Kistler amplifier 9017 and a NI Labview acquisition system. The thickness \(w\)
is equal to $318 \mu m$. For the trials, the selected cutting speeds are 60 m/min and 90 m/min. The experiments are carried out to observe the effects of feed, varying from 5 to $40 \mu m$/rev. To perform orthogonal micro-cutting tests, the cutting edge axes has to cross the tube axes. Each test corresponds to 10 revolutions. Cutting conditions are considered stable and did not influence the experimental tests. Each cutting condition was repeated at least 3 times.

Figure 3 shows a force signals obtained when micro-cutting the Ti42Nb specimens with a feed of $20 \mu m$/rev. Force signals $F_x$, $F_y$ and $F_z$, correspond respectively to the cutting force $-F_c$, the passive force $F_p$ and the feed force $F_f$. Orthogonal cutting conditions are validated, $F_y$ signal being equal to 0. Cutting forces $F_x$ and $F_z$ rise during 0.016s corresponding to one rotation of the tube. Then, a stable value is reached. An average value of the cutting force response is extracted for various cutting condition and reported in results section, figures 11 and 12.


3 Numerical modeling

3.1 Kinematics

Using the material point motion history function $\chi$, the motion of a single crystal in the deformed configuration is expressed as follows:

$$x = \chi(X, t)$$  \hspace{1cm} (1)

where $t$ and $X$ are the time and the position of the material point in the reference configuration, respectively. The deformation gradient tensor $F$ is expressed from the motion history function according to:

$$F(X, t) = \frac{\partial \chi}{\partial X}$$  \hspace{1cm} (2)

Following Lee [17], a multiplicative decomposition of the deformation gradient tensor $F$ is adopted in this work:

$$F = F_\theta \cdot F_d \cdot F_p$$  \hspace{1cm} (3)

Here, $F_\theta$ and $F_p$ are the thermoelastic and plastic contributions to deformation gradient $F$. $F_d$ represents the contribution to deformation gradient due to damage propagation. Therefore, $F_d$ can be written as:

$$F_d = (1 + AD)I$$  \hspace{1cm} (4)

where, $A$ is a parameter that controls the contribution damage to deformations and $D$ is the damage variable.

The concept of the isoclinic intermediate configuration suggested by Mandel [21] is used to formulate the constitutive equations. Four different configurations are introduced (see Figure 4): The initial configuration $C_0$, the isoclinic intermediate configuration $\tilde{C}$, the damaged configuration $\hat{C}$ and the current configuration $C_t$. The impact of microstructure features on the orthogonal micro-cutting response is considered using framework of crystal plasticity. For metallic materials, the general framework of crystal plasticity provides a convenient method to incorporate the role of microstructural heterogeneities or anisotropy. The deformation gradient tensor $F$ allows to define the Green-Lagrange strain tensor $E$ that characterize the deformation state of the single crystal from:

$$E = \frac{1}{2} \left( F^T \cdot F - I \right)$$  \hspace{1cm} (5)
Fig. 4 Kinematics of single crystal showing the decomposition of the deformation gradient tensor $\mathbf{F}$ into a thermoelastic part $\mathbf{F}_\theta$, a damage-induced part $\mathbf{F}_d$ and a plastic part $\mathbf{F}_p$.

The thermoelastic, the plastic and the damage-induced contributions to the deformations are given by:

$$
\tilde{\mathbf{E}}_\theta = \frac{1}{2} (\mathbf{F}_\theta^T \cdot \mathbf{F}_\theta - \mathbf{I})
$$

$$
\mathbf{E}_p = \frac{1}{2} (\mathbf{F}_p^T \cdot \mathbf{F}_p - \mathbf{I})
$$

$$
\hat{\mathbf{E}}_d = \frac{1}{2} (\mathbf{F}_d^T \cdot \mathbf{F}_d - \mathbf{I})
$$

Here, $\mathbf{E}$ and $\mathbf{E}_p$ are attached to the initial configuration. However, the thermoelastic deformation tensor $\tilde{\mathbf{E}}_\theta$ and the damage-induce deformation tensor $\hat{\mathbf{E}}_d$ are expressed in the intermediate configuration $\hat{\mathbf{C}}$ and the current configuration $\mathbf{C}_t$, respectively. Using the thermoelastic $\mathbf{F}_\theta$ and plastic $\mathbf{F}_p$ parts of the deformation gradient tensor, the total strain tensor $\mathbf{E}$ is given by:

$$
\mathbf{E} = \mathbf{E}_p + \mathbf{F}_p^T \cdot \tilde{\mathbf{E}}_\theta \cdot \mathbf{F}_p + \mathbf{F}_p^T \cdot \hat{\mathbf{E}}_d \cdot \mathbf{F}_\theta \cdot \mathbf{F}_p
$$

Similarly, the velocity gradient tensor $\mathbf{L}$ can be defined as follows:

$$
\mathbf{L} = \dot{\mathbf{F}} \cdot \mathbf{F}^{-1}
$$
By injecting the equation (3) into the previous equation, the velocity gradient tensor \( \bar{L} \) is expressed as:

\[
\bar{L} = \dot{F}_d \cdot F_d^{-1} + F_d \cdot \dot{\theta}_\theta \cdot F_\theta^{-1} \cdot F_d^{-1} + F_d \cdot \dot{\theta}_\theta \cdot \dot{F}_p \cdot F_p^{-1} \cdot F_\theta^{-1} \cdot F_d^{-1}
\]  

(11)

The velocity gradient tensor \( \bar{L} \) is decomposed into a thermoelastic part \( \bar{L}_\theta \), a damage-induced part \( \bar{L}_d \) and a plastic part \( \bar{L}_p \) as follows:

\[
\bar{L} = \bar{L}_d + \bar{L}_\theta + \bar{L}_p
\]  

(12)

here,

\[
\bar{L}_d = \dot{F}_d \cdot F_d^{-1}
\]  

(13)

\[
\bar{L}_\theta = F_d \cdot \dot{\theta}_\theta \cdot F_d^{-1}
\]  

(14)

\[
\bar{L}_\theta = \dot{\theta}_\theta \cdot F_\theta^{-1}
\]  

(15)

\[
\bar{L}_p = F_d \cdot \dot{\theta}_\theta \cdot \tilde{L}_p \cdot F_\theta^{-1} \cdot F_d^{-1}
\]  

(16)

\[
\bar{L}_p = F_p \cdot F_p^{-1}
\]  

(17)

while \( \tilde{L}_p \) and \( \tilde{L}_\theta \) are attached respectively to the intermediate and current configurations. \( \bar{L} \) and \( \bar{L}_d \) are related to the damaged current configuration.

### 3.1.1 State equations

In order to model the evolution of material point during the micro-cutting process, constitutive equations must be specified. In this work, a hyperelastic constitutive model is developed. Based on the concept of the thermodynamically consistent formulation, some state variables are adopted to describing the constitutive equations. These state variables are the thermoelastic strain tensor \( \tilde{E}_\theta \), the temperature \( T \), the isotropic hardening variables \( q_s \) associated with each slip system \( s \) and the damage variable \( D \). Furthermore, the state variables allow to define the state potential \( \psi \) as follows:

\[
\bar{\psi} \left( \tilde{E}_\theta, q_s, T, D \right) = \bar{\psi}_\theta \left( \tilde{E}_\theta, T, D \right) + \bar{\psi}_T (T) + \bar{\psi}_p (q_s, T, D)
\]  

(18)

where \( \bar{\psi}_\theta \), \( \bar{\psi}_T \) and \( \bar{\psi}_p \) denote respectively the thermoelastic contribution, the thermal contribution and the contribution due to the isotropic hardening. These contributions depend on the damage variable \( D \) in order to obtain an elastic/damage coupling and a hardening/damage coupling. The specific free energy \( \bar{\psi} \) is expressed in the intermediate configuration as follows:

\[
\bar{\psi} = \frac{1}{2} \tilde{E}_\theta : C (D) : \tilde{E}_\theta - \tilde{E}_\theta : C (D) : \alpha (T - T_0) + \bar{c} (T - T_0 - T \ln \left( \frac{T}{T_0} \right))
\]
\[ + \frac{1}{2} \alpha : (C(D) - C_0) : \alpha (T - T_0)^2 + \frac{1}{2} Q (1 - D) \sum_s q_s \sum_t h_{st} q_t \quad (19) \]

where, \( T_0, c, Q, \) and \( h_{st} \) denote respectively the reference temperature, the specific heat, the isotropic hardening moduli and the interaction matrix between the different slip systems. \( \alpha \) is the thermal expansion tensor at room temperature. \( C(D) \) and \( C_0 \) are respectively the current stiffness tensor that depends on the damage variable \( D \) and the initial undamaged stiffness tensor that account for the anisotropy of the BCC structures. The current stiffness tensor is expressed as follows [10]:

\[
C(D) = \begin{cases} 
C_t, & \text{tr}[E_e] > 0 \\
C_t + P_s : (C_0 - C_t) P_s, & \text{tr}[E_e] \leq 0 
\end{cases} \quad (20)
\]

with

\[
C_t = \left[ C_0^{-1} + g(D) \left( A_s P_s : C_0^{-1} : P_s + A_d P_d : C_0^{-1} P_d \right) \right]^{-1} \quad (21)
\]

In the equation (20), \( E_e = E_\theta - \alpha (T - T_0) \) is the elastic deformations tensor. \( P_s \) and \( P_d \) are respectively the spherical and the deviatoric projection tensors defined as follows:

\[
P_s = \frac{1}{3} I \otimes I \quad (22)
\]

\[
P_d = I - \frac{1}{3} I \otimes I \quad (23)
\]

In the equation (21), two material parameters \( A_s \) and \( A_d \) are introduced to control the contributions of spherical and deviatoric parts of strains to damage development. \( g(D) \) is degradation function given by:

\[
g(D) = \frac{D}{1 - D} \quad (24)
\]

The specific Helmholtz free energy \( \psi \) can be used to obtain the state equations. In this work, a thermodynamic force is associated with each state variable [10]. These forces are the second Piola-Kirchoff stress tensor \( \tilde{P} \), the specific entropy \( S \), the critical shear stress \( R_s \) and the driving force for damage \( Y \). The list of state variables as well as the associated thermodynamic forces used in this work is presented in the Table 2.

Therefore, it is possible to obtain the state equations which connect the driving forces to their state variables from a state potential. The second Piola-Kirchoff \( \tilde{P} \) stress tensor is obtained using the equation (19) as follows:

\[
\tilde{P} = \rho \frac{\partial \psi}{\partial \tilde{E}_\theta} = C(D) : \left( \tilde{E}_\theta - \alpha (T - T_0) \right) \quad (25)
\]
Table 2 State variables and associated thermodynamic forces used to characterize the state of the material point.

<table>
<thead>
<tr>
<th>State variables</th>
<th>thermodynamic forces</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T$</td>
<td>$S$</td>
</tr>
<tr>
<td>$\tilde{E}_\theta$</td>
<td>$\tilde{P}$</td>
</tr>
<tr>
<td>$q_s$</td>
<td>$G_s$</td>
</tr>
<tr>
<td>$D$</td>
<td>$Y$</td>
</tr>
</tbody>
</table>

The thermodynamic force $Y$ resulting in the development of the damage $D$ is given by:

$$Y = -\varrho \frac{\partial \psi}{\partial D} = -\frac{1}{2} \tilde{E}_\theta : \tilde{E}_\theta + \frac{1}{2} Q \sum_s q_s \sum_t h_{st} q_t$$  \hspace{1cm} (26)

The critical shear stress $R_s$ measures the resistance to the plastic slip for each sliding system $s$ is written as follows:

$$R_s = \varrho \frac{\partial \psi}{\partial q_s} = (1 - D) Q \sum_t h_{st} q_t$$  \hspace{1cm} (27)

The specific entropy $S$ is expressed from the specific free energy as follows:

$$\varrho S = -\varrho \frac{\partial \psi}{\partial T} = -\frac{1}{2} \tilde{E}_\theta : \frac{\partial C}{\partial T} : \tilde{E}_\theta + \tilde{E}_\theta : \frac{\partial C}{\partial T} : \alpha (T - T_0)$$

$$+ \tilde{E}_\theta : C : \alpha - \frac{1}{2} \alpha : \frac{\partial C}{\partial T} : \alpha (T - T_0)^2$$

$$- \alpha : (C - C_0) : \alpha (T - T_0)$$

$$+ c \ln \left[ \frac{T}{T_0} \right] - \frac{1}{2} \frac{\partial Q}{\partial T} (1 - D) \sum_s q_s^\phi \sum_t h_{st}^\phi q_t$$  \hspace{1cm} (28)

### 3.1.2 Specific dissipation

Because thermodynamic principles lead to some restrictions on the development of constitutive equations, these equations are briefly recalled in the following section. First, the first principle of thermodynamics postulates that the total energy can only change under the effect of mechanical and thermal energy. The local form of the first principle is given by:

$$\varrho \dot{U} = \Pi : \dot{F} + \varrho r - \text{div} (q)$$  \hspace{1cm} (29)

where $U$ is the specific internal energy, $r$ and $q$ are respectively the heat flux density vector and the specific heat source.

Second, the second law of thermodynamics requires that the entropy production is non-negative. The local form of the second law is given by the
following inequalities:
\[
\varrho \dot{S} - \varrho \frac{r}{T} + \text{div} \left( \frac{q}{T} \right) \geq 0 \tag{30}
\]
where \( S \) is the specific entropy. \( r/T \) and \( q/T \) are respectively the entropy source and the entropy flux vector. The specific dissipation source \( d_i \) can be obtained by the product of the equation (30) by the absolute temperature \( T \). The expression of the specific dissipation source \( d_i \) is written as follows:
\[
d_i = \varrho T \dot{S} - \varrho r + \text{div} (q) \geq 0 \tag{31}
\]
The intrinsic dissipation source \( d_1 \), which represents the part of the work received and converted locally into heat, is given by [11]:
\[
d_1 = \varrho T \dot{S} - \varrho r + \text{div} (q) \geq 0 \tag{32}
\]
The thermal contribution due to conduction transfers is written as:
\[
d_2 = - \frac{q \cdot \nabla T}{T} \geq 0 \tag{33}
\]
Based on the work of Germain et al. [11], one can assume the separation between \( d_1 \) and \( d_2 \), and the non-negative of each of them in order to be compatible with the second law of thermodynamics. The specific free energy \( \psi \) can be expressed as a function of the internal energy, the temperature and specific entropy as follows:
\[
\psi = U - TS
\]
Using the time derivation of the free energy, the equation of the first principle (29) and the equation of the intrinsic dissipation (32), the intrinsic dissipation can be written in the following form:
\[
d_1 = \dot{\Pi} : \dot{U} - \varrho \dot{\psi} - \varrho \dot{T} s
\]
Using the expression of the specific free energy (19), one can get:
\[
d_1 = \frac{1}{\varrho} \left( \tilde{M} : \tilde{L}_p - \sum \limits_s R_s \dot{q}_s - Y \dot{D} \right) \tag{35}
\]
In the equation (35), the Mandel stress tensor \( \tilde{M} \), which represents the thermodynamic force associated with \( \tilde{L}_p \), is introduced. This stress tensor which is attached to the isoclinic intermediate configuration is related to the second Piola-Kirchhoff \( \tilde{P} \) stress tensor with:
\[
\tilde{M} = F^T_{\theta} \cdot F_{\theta} \cdot \tilde{P} \tag{36}
\]
Therefore, the resolved shear stress $\tilde{\tau}_s$ associated with the slip system $s$ is expressed from the Mandel stress tensor as follows:

$$\tilde{\tau}_s = \tilde{t}_s \cdot \tilde{M} \cdot \tilde{n}_s$$

(37)

The equation (35) shows that, to complete the description of the constitutive model, it is necessary to define some evolution laws for $\tilde{L}_p$ and $\dot{\gamma}_s$.

### 3.1.3 Evolution laws

Based on the crystal plasticity framework, the plastic part of the velocity gradient tensor is given by:

$$\tilde{L}_p = \sum_s \dot{\gamma}_s \tilde{t}_s \otimes \tilde{n}_s$$

(38)

where $\dot{\gamma}_s$ is the plastic shear strain rate on the slip system $s$. In the following, the Méric and Cailletaud [22] work is used to build the evolution law of the plastic shear strain.

$$\dot{\gamma}_s = \bar{\upsilon}_s \text{sign} (\tilde{\tau}_s)$$

(39)

$\bar{\upsilon}_s$ is the average velocity on the slip system $s$ which can be expressed as a function of the resolved shear stress $\tilde{\tau}_s$ from a power law with:

$$\bar{\upsilon}_s = \left< \frac{|\tilde{\tau}_s| - R_s}{K} \right>^n$$

(40)

$K$ and $n$ are viscoplastic flow rule parameters. By injecting the equation (40) into the equation (39), one can obtain:

$$\dot{\gamma}_s = \left< \frac{|\tilde{\tau}_s| - R_s}{k} \right>^n \text{sign} (\tilde{\tau}_s)$$

(41)

The saturated hardening model proposed by Méric and Cailletaud [22] is adopted in this work to describe the isotropic hardening. It is given by:

$$\dot{q}_s = (1 - bq_s) \left| \dot{\gamma}_s \right|$$

(42)

where the isotropic hardening saturation is controlled by the parameter $b$. Initially, the material contains an amount of dislocations, a non-zero initial value of $q_s$ is considered. The equation (42) becomes:

$$\dot{q}_s = (1 - bq_s) \left| \dot{\gamma}_s \right| \quad \text{and} \quad q_s(t = 0) = q_0$$
To describe the degradation of the material properties during micro-cutting, the evolution of the damage variable is modelled using a power-law:

$$\dot{D} = \left( \frac{Y}{Y_0} \right)^m \|\tilde{L}_p\| (1 - D)$$  \hspace{1cm} (43)

In the above equation, $Y_r$ and $m$ are material parameters controlling the rate of damage accumulation.

This model is implemented in the ABAQUS/Explicit finite element solver with a user-defined subroutine. This subroutine allows to delete elements in the finite element analysis when the damage variable is greater than 0.99, indicating the degradation of the mechanical properties in the polycrystalline Ti42Nb alloy. The model proposed in this sections introduce mechanical and thermophysical parameters that need to be adjusted. In the next section, the adjustment was performed using experimental results obtained on compression tests. Furthermore, these parameters are identified from experimental tests conducted under two strain rates and a width range of temperatures.

3.2 Parameter identification

Some mechanical and thermophysical parameters introduced to formulate the constitutive equations, are obtained in part from literature data.

For the BCC Ti42Nb, the plastic slip is considered to occur on the 24 slip systems $\langle 111 \rangle \{110\}$ and $\langle 111 \rangle \{112\}$ [23, 18, 19]. For such choice of slip systems, the interaction matrix $h$ is formed by 576 coefficients. In this work, for each slip system $s$, the self-hardening and the latent hardening are equivalent which means to set the coefficients of the interaction matrix $h$ to unit. Heat transfers are not considered and the tests are adiabatic. In order to use the proposed constitutive model during micro-cutting simulations, it is necessary to identify the parameters of viscoplastic flow rule, isotropic hardening law and damage rule listed in Table 3.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Viscoplastic flow rule $K$ and $n$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isotropic hardening rule</td>
<td>$Q$, $b$ and $q_0$</td>
</tr>
<tr>
<td>Damage rule</td>
<td>$A$, $A_d$, $A_s$, $Y_r$ and $m$</td>
</tr>
</tbody>
</table>

Table 3  Viscoplastic, isotropic hardening and damage parameters.
In the following, an inverse method is used to identify the material parameters of the proposed model. The results obtained from the uniaxial compression tests were used to adjust the parameters of the viscoplastic flow rule, the isotropic hardening rule and the damage rule. To perform the inverse method, the proposed model is implemented within the ABAQUS Explicit finite element solver. Figure 5 shows the numerical model adopted to simulate the uniaxial compression tests. Since the size of the $\beta$ grain is about 80 $\mu$m, each finite element is considered as a single grain.

**Fig. 5** Geometrical model and boundary conditions adopted for the simulation of uniaxial compression tests.
Figure 6 shows the numerical and experimental nominal stress versus nominal strain curves obtained after parameter identification. As illustrated in figure 6, the temperature impacts greatly the flow stress and the fracture strain of the alloy. For a given strain rate, the flow stress decreases and the elongation to fracture increases as the temperature increases. It is important to highlight that the flow stress drops drastically when the temperature is increased from 298 K to 673 K. According to the results (see Figure 6), a good agreement with experimental results is obtained. Specifically, the decrease of the hardening rate and the ultimate yielding stress with an increasing temperature is correctly depicted.
Figure 7-c shows an experimental observation of Ti42Nb specimen deformed at a strain rate of 10 s$^{-1}$ and a temperature of 25°C. According to the observation, a strain localization mode impacts the deformation behavior of the alloy. Specifically, the localization of the plastic deformation, which is observed at room temperature, leads to the formation of an Adiabatic Shear Band (ASB). Figure 7-a illustrates that a numerical simulation with the same loading conditions. According to the results, the numerical simulation is consistent with the experimental findings. As shown in Figure 7-b, a shearing band oriented with an angle of ±45° with respect to the compression direction, is obtained. Indeed, the numerical result indicates that the crack initiation sites are the two tips of the shear band. The formation of the shear band is mostly explained by both the softening behavior of the alloy and the local temperature rise (see Figure 7-d), which reaches high value (477 K) at the instance of fracture.

3.3 Orthogonal micro-cutting

3.3.1 Impact of cutting parameters

In the following, the proposed model is validated by comparing the numerical cutting forces with the experimental results. Orthogonal micro-cutting experiments are conducted with different feed rates ($f = 5, 10, 20$ and $40$ mm/rev) and two cutting speeds ($V_c = 60$ and $90$ m/min). A 3-dimensional
finite element cutting model is proposed and includes a rigid cutting tool and an BCC polycrystalline workpiece with the 24 potentially active systems. The geometrical model and the boundary conditions adopted for orthogonal cutting simulations are shown in Figure 8. The polycrystalline \( \beta \) titanium alloy workpiece contains non-columnar elongated \( \beta \)-grains with average size of 80 \( \mu m \) and specific crystallographic orientations. The workpiece is divided into different regions. The first region represents the cutting domain (500 \( \times \) 200 \( \times \) 150 \( \mu m^3 \)) is meshed with uniform C3D8RT elements with mesh size about (10 \( \times \) 4 \( \times \) 10 \( \mu m^3 \)). A second domain, which is not machined, is meshed with non-uniform C3D8RT elements in order to reduce the computation costs. A Coulomb friction law is used to model the friction at the tool/chip interface. The friction coefficient of 0.2 is under-estimated for the cutting simulations comparing to the friction coefficient calculated using the experimental cutting and thrust forces data. The parameters identified from compression test and used to formulate the constitutive equations are used in the cutting simulations of the polycrystalline Ti42Nb alloy.

In this work, the experimental and numerical average values of the cutting forces \( F_c \) and the feed forces \( F_f \) are compared. The numerical cutting forces are plotted in Figure 9 for the cutting forces \( F_c \) and in Figure 10 for the feed forces \( F_f \). In the following, because the experimental and numerical cutting depth are different, the cutting forces are assumed to vary linearly with the cutting depth. As a result, the numerical cutting force is converted and compared to the experimental results. As shown in Figure 9, an increase of the feed rates...
or a decrease of the cutting speed is associated with an increase of the cutting forces $F_c$. According to the result, the effect of the cutting velocities and the feed rates on the cutting forces response of the Ti42Nb titanium alloy produced by laser-based powder bed fusion is correctly depicted. The error between the numerical and the experimental cutting forces $F_c$ does not exceed 10%.

![Comparison between numerical and experimental cutting forces](image.png)

**Fig. 9** Comparison between the numerical and experimental cutting forces $F_c$ obtained under different cutting velocities and feed rates.

The impact of the cutting velocity on the cutting forces can be related to the strain softening of the alloy. As shown in figure 6, the temperature impacts strongly the flow stress of the alloy. An increase of the initial temperature from 25° to 400° is associated with a drop of the flow stress from 1100 MPa to 460 MPa. Since, the majority of the plastic work is converted locally into heat which produces an elevation of the workpiece temperature, the increase of the cutting velocity from 60 to 90 m/min leads to enhance the plastic dissipation and therefore the rise of the local temperature. The latter reduces the flow stress and consequently the cutting forces.
Figure 10 illustrates the effect of the cutting velocities and the feed rates on the feed forces $F_f$. According to the result, the impact of cutting parameters on the feed forces is largely under-estimated. The error between the numerical and the experimental feed forces $F_f$ almost exceed 30%. The proposed model is not able to reproduce the feed forces $F_f$ when cutting the Ti42Nb titanium alloy produced by laser-based powder bed fusion. The above problem can be related to the ductility of the alloy that enhances the feed forces $F_f$. Therefore, the choose of a Coulomb friction law to model the friction at the tool/chip interface with a friction coefficient of 0.2 is not efficient for the above cutting simulations. However, increasing the friction coefficient leads to mesh distortion problem in the case of Lagrangian formulation.
Fig. 11 Evaluation of instantaneous local variables (equivalent plastic deformation gradient field $\|\mathbf{E}^p\|$, damage filed $D$, and temperature field $T$) at the instant of cutting for Ti42Nb specimen.

Fig. 12 Evaluation of instantaneous local variables (equivalent plastic deformation gradient field $\|\mathbf{E}^p\|$, damage filed $D$, and temperature field $T$) at the instant of cutting for Ti42Nb specimen.

For the purpose of evaluating the impact of the local microstructure on micro-cutting response, Ti42Nb workpiece material is investigated. Indeed, the same 3-dimensional finite element cutting model is used in this section. Orthogonal micro-cutting simulations are performed with a cutting velocity and feed
rate of 60 m/min and 50 µm respectively. The average grains size is 80 µm. Figures 11 and 12 show the evaluation of instantaneous local variables (equivalent plastic deformation gradient field $\|E_p\|$, damage field $D$, and temperature field $T$) at the instant of micro-cutting for Ti42Nb specimen on the two lateral surfaces. According to the results, the morphology of the formed chip on the two lateral surfaces of the workpiece is different. Adiabatic shear bands are clearly observed in Figure 11 with a localisation of the plastic deformation and temperature in these zones. However, as shown in Figure 12, the temperature and the plastic deformation are concentrated in the tool-chip interaction zone.

3.3.2 Impact of crystallographic orientation
In the following, the impact of the local texture on the micro-cutting response of Ti42Nb alloy is evaluated. Indeed, a 3-D finite element micro-cutting model is used in this section. Orthogonal micro-cutting simulations are performed with a cutting velocity of 60 m/min and feed rate of 50 µm. For the purpose of evaluating the impact of the crystallographic orientation on the chip formation, the cutting direction (that corresponds to the X-axis in figure 8) is oriented in all grains respectively according to the directions [100], [101] and [111]. The evaluation of instantaneous local variables (equivalent plastic deformation gradient field \(\|E_p\|\), damage filed \(D\), and temperature field \(T\)) at the instant of micro-cutting for Ti42Nb specimen are shown in Figure 13. According to the results, the crystallographic orientation impacts strongly the thickness and the morphology of the formed chip. The highest chip thickness is obtained for the cutting direction oriented [100] in all grains while the lowest chip thickness is observed when cutting along the [111] direction. For the two cutting direction, a continues chip morphology is obtained. However, when the cutting direction \(\vec{V}_c\) is parallel to [101] direction the morphology of the formed chip is slightly segmented and shows the formation of the adiabatic shear band largely observed when machining titanium alloy. When adiabatic shear bands are formed, the plastic deformation is localised in these narrow zones which leads to the initiation and the propagation of the damage. However, when cutting parallel to the [100] and [111] directions the plastic deformation are localised in the chip-tool interface zone that leads to increase the local temperature in this zone (see Figure 13 a and c).

**Fig. 13** Evaluation of instantaneous local variables (equivalent plastic deformation gradient field \(\|E_p\|\), damage field \(D\), and temperature field \(T\)) for Ti42Nb specimen with a) \(\vec{V}_c\) parallel to [100] b) \(\vec{V}_c\) parallel to [101] and c) \(\vec{V}_c\) parallel to [111].
3.3.3 Impact of grain size

In this section, the impact of the grain size on micro-cutting response of Ti42Nb alloy is investigated using the same finite element cutting model. Orthogonal micro-cutting simulations are performed with a cutting velocity of 60 m/min and feed rate of 50 µm. For the purpose of evaluating the impact of the grain size on the chip formation, three simulations are performed with 7, 70 and 300 β-grains respectively. Evaluation of instantaneous local variables
(equivalent plastic deformation gradient field $\|E^p\|$, damage filed $D$, and temperature field $T$) at the instant of micro-cutting for Ti42Nb specimen are shown in Figure 14. According to the results, the grain size impacts greatly the chip morphology. A continuous chip is obtained for the micro-cutting simulations performed on workpiece that contains 7 grains, while a slightly segmented chip and a totally segmented chip are obtained for the workpieces contain 70 grains and 300 grains, respectively. Also, an increase of the grain size is associated with an increase of the chip thickness. When the grain size is decreased the formation of the adiabatic shear bands is more pronounced. This effect can be explained through the average effect of the crystallographic orientation when the grain size is decreased. Finally, increasing the grain size is associated with a localization of the temperature at the tool-chip interface.

4 Conclusions

In this work, experimental and numerical investigations have been conducted to investigate the micro-cutting response of as-additive manufacturing Ti42Nb titanium alloy produced by laser-based powder bed fusion. Experimental micro-cutting trial are conducted with two cutting velocities (60 m/min and 120 m/min) and different feed rates (5, 10, 20 and 40 $\mu$m/rev). For the numerical investigations, a crystal plasticity based model has been developed and implemented in the ABAQUS/Explicit finite element solver with a user-defined subroutine. The model has been identified using strain–stress curves obtained from compression tests performed under two strain rates and a wide range of temperatures. The crystal plasticity-based model is used in order to perform numerical micro-cutting simulations to gain insight into the impact of microstructural features (i.e. crystallographic orientation and grain size) on the machinability of the alloy. According to the results, the effect of cutting parameters on the machining response in term of cutting forces of the Ti42Nb titanium alloy produced by laser-based powder bed fusion is correctly depicted. In addition, the local variables such as temperature, damage and plastic deformation are strongly impacted by the crystallographic orientations and the grain size. Depending on the crystallographic orientations, the chip morphology changes from continues, slightly segmented to largely segmented.

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