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▶ To cite this version:

Hannah Lois Dorothy, Patrice Longère. Unified modelling of adiabatic shear banding and subsequent micro-voiding driven dynamic failure of viscoplastic solids. International Journal of Impact Engineering, 2019, pp.103322. 10.1016/j.ijimpeng.2019.103322. hal-02159745

HAL Id: hal-02159745 https://hal.science/hal-02159745

Submitted on 25 Oct 2021

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Unified modelling of adiabatic shear banding and subsequent micro-voiding driven dynamic failure of viscoplastic solids

Hannah Lois Dorothy^a, Patrice Longère^a

^aUniversité de Toulouse, UT3-UPS, ISAE-SUPAERO, Institut Clément Ader (CNRS 5312), 3 rue Caroline Aigle, 31400 TOULOUSE, France

8 ABSTRACT

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9 Adiabatic shear bands (ASBs) are intense shear localisation zones resulting from 10 thermomechanical instability in dynamically loaded, high strength structural materials. In the wake of the ASB, Micro-voids (MVs) have been observed which coalesce and 11 ultimately rupture the material. ASBs thus favour premature MV induced damage and 12 further material failure. In the present work, the coupled effects of ASB+MV on the 13 representative volume element (RVE) are reproduced in a unified model within 14 irreversible thermodynamics framework considering a large scale postulate. The 15 influence of the softening mechanisms such as thermal softening and/or DRX induced 16 softening on the ASB onset is accounted for. The model is numerically implemented as a 17 18 user material subroutine into the engineering finite element (FE) computation code LS-DYNA and its feasibility and performances are assessed on both RVE and structural 19 20 scales. The dynamic shear compression loading of a hat shaped structure is simulated 21 for that purpose. The respective contributions of ASB and MV on the progressive 22 material deterioration can be clearly identified.

23 Keywords:

24 Adiabatic shear banding, Ductile damage, Dynamic plasticity, Numerical simulation

25 1 INTRODUCTION

26 The present study aims at modelling the adiabatic shear banding and the consecutive 27 micro-voiding induced material deterioration. Adiabatic shear banding is a distinct 28 deformation mechanism which occurs in viscoplastic solids during high strain rate and 29 impact loading acting as a precursor to failure such as plugging failure, ductile fracture, 30 explosive failure, etc., see [1],[2],[3]. The Adiabatic Shear Bands (ASBs) are seen 31 typically in high strength metals and alloys such as steels and titanium and aluminium alloys which are often used as component materials for aircraft and other structures. 32 33 The ASBs are undesirable when they cause catastrophic failures of structures such as 34 protection plates for ballistic applications [4] involving military or civil threats (missile, 35 bird strike, etc). On the other hand, they are desirable in military application such as 36 kinetic energy penetrators in which the formation of ASBs on the side ends of the 37 penetrator helps in a self-sharpening-like mechanism ([5],[6],[7]). They also find 38 industrial application in high speed machining in which they have mitigated effect in the 39 sense that they help to reduce the cutting force but at the expense of cutting force 40 oscillation and rougher surface finish [8], [9]. In the context of engineering design, it is 41 thus crucial to be able to numerically reproduce the consequences of this phenomenon.

The ASBs are narrow regions of intense plastic shear deformation and strength 42 43 softening resulting from thermo-mechanical instability induced by a competition 44 between hardening and softening mechanisms in the regions of low stress triaxiality 45 during high strain rate loading. The mechanisms causing the softening which triggers 46 the ASB formation are mostly plastic dissipation-induced temperature rise and possibly 47 dynamic recrystallization (DRX) in certain materials. The shear bands are distinctly 48 oriented causing local degradation of the material properties and a form of induced 49 anisotropy at the scale of the specimen. Once the ASB is formed, the softer material 50 within the band serves as a site for the nucleation and growth of micro-voids (MV). 51 These micro-voids additionally contribute to softening mechanism and accelerate the 52 post-localization drop in strength of the RVE in the large scale postulate framework. The 53 micro-voids coalesce and lead to the formation of cracks which ultimately fracture the 54 material. The evidence of the presence of micro-voids within the ASB was shown by 55 various experimental observations ([10],[2],[11]). The experimental observation 56 reported in on the fracture surface of impacted shear compression specimens showed the evidence of micro-voids in the ASB wake which proved that the fracture occurred 57 58 due to two successive mechanisms: adiabatic shear banding and then micro-voiding.

59 The ASB in itself is a weak discontinuity, causing shape change, as there is cohesion of matter within the band; the MV is a strong discontinuity with the absence of matter 60 within, creating irreversible damage in the material and imposing volume change and 61 related hydrostatic components to the induced strain rate because of the void growth. 62 63 Depending on the loading, the ASB does not necessarily lead to micro-voiding and 64 further failure; and in certain cases, upon unloading, the ASB is quenched by the cooler 65 surrounding material, undergoes phase transformation and finally becomes harder at 66 room temperature than the surrounding matrix material [12]. Therefore considering a 67 unique variable accounting indistinctly for ASB and MV does not allow for distinguishing 68 the zones in the structure where ASB takes place, with potential initial properties 69 recovering after unloading and cooling as explained above, and where irreversible void-70 growth induced irreversible damage as a precursor to crack formation takes place. Being 71 able to distinguish the respective contributions of ASB and MV on the current (during

loading) and residual (post loading) material deterioration is accordingly of majorinterest.

74 Many approaches describing the ASB in the literature are developed at a scale lower 75 than the bandwidth ([13], [14] and [15]). However, as the ASB width in itself is of the 76 order of micro-meters, this postulate requires the use of very fine meshing in the finite 77 element (FE) simulations. Whereas in the present study, a large scale postulate is adopted, in which the representative volume element (RVE) has a length scale greater 78 79 than the ASB width; in other words, the shear band is embedded within the RVE. This approach facilitates the use of coarser meshes in FE simulations and thus makes the 80 81 model feasible to implement on engineering structural applications. Large scale approaches based on variational methods and enriched finite elements can be found in 82 83 [16], [17], [18] and [19], and a review of ASB-oriented modelling approaches in [20]. 84 While modelling of ASB can be widely found in the literature, the subsequent mechanism 85 of micro-voiding and its modelling as a distinct contribution to the failure process is 86 largely overlooked. The present work aims to model in a unified approach the ASB and 87 subsequent MV induced degradation.

88 A physics motivated phenomenological three-dimensional constitutive model was 89 initially developed by Longère et al. [21] in an irreversible thermodynamics framework which described the material degradation induced predominantly by the ASB. The aim 90 91 here is to use an enlarged version of the aforementioned model based on the model 92 developed recently by Longère and Dragon [22] in order to explicitly reproduce the 93 consequences of micro-voiding in the band wake. The view is to clearly distinguish in 94 the post-critical regime the respective contributions to the material softening coming 95 from the two mechanisms at stake, namely adiabatic shear banding on one hand and micro-voiding on the other hand. The ASB+MV model is here implemented as user 96 97 material into the engineering finite element (FE) computation code LS-DYNA in the context of standard FE kinematic formulation. The numerical feasibility of the enriched 98 99 model and the results showing the distinct ASB and MV effects are then demonstrated 100 on the RVE and structural scales.

Section 2 presents the development of the constitutive model. The numerical issues encountered in the finite element implementation and performance of enriched ASB+MV model is assessed by numerical implementation on RVE scale and initial boundary value problems (IBVP) in Section 3. Finally the conclusions are drawn in Section 4 and some prospective work is suggested.

106 2 BASIC CONCEPTS AND CONSTITUTIVE MODELLING

The physical aspects and mechanical consequences of ASB and MV are presented below
followed by the development of the constitutive model in an irreversible
thermodynamics framework.

110 2.1 PHYSICAL AND MECHANICAL ASPECTS

111 The high strength metals and alloys under high strain rate loading first exhibit elasto-112 plasticity. During this stage, the self-heating caused by plastic dissipation and/or 113 softening due to dynamic recrystallization may lead to the formation of a localized shear 114 deformation (ASB) which causes material strength deterioration and alters the 115 kinematics of the plastic flow. Further, damage is encountered within the shear bands 116 causing the material failure. The scenario for ASB and MV assisted failure which is 117 considered for modelling in the present study and their effects on the shear stress-shear strain curve are depicted in Fig. 1. The regular mechanism of polycrystalline plasticity is 118 119 in action during the initial stage of hardening. Then the formation of the ASB reduces the 120 material strength. The drop in the material strength in the post critical stage is 121 potentially accelerated by the formation of micro-voids in the wake of the ASB. The 122 micro-voids coalesce and ultimately rupture the material.





126 In the following subsections, the salient physical and mechanical features involved are127 presented.

128 2.1.1 Physical considerations

- 129 The physical features and the formation process of the adiabatic shear bands and micro-
- 130 voids are presented in this section.
- 131 2.1.1.1 Adiabatic shear banding

132 As mentioned above, the ASBs are distinctly oriented shear localizations resulting from a 133 thermo-mechanical instability phenomenon. The heat produced from the plastic deformation during high strain rate loading, when not having enough time to be 134 135 conducted away leads to local increase in temperature giving rise to a 'quasi-adiabatic' 136 condition. This causes a local thermal softening of the material. Thermo-mechanical 137 instability comes into play as a competition arises between the thermal softening and 138 strain or/and strain-rate hardening. When the rate of this thermal softening surpasses 139 the strain/strain rate hardening, the material deformation becomes unstable and 140 concentrates in narrow softened bands which are termed as ASBs. This widely accepted 141 mechanism of ASB inception and growth was first proposed by Zener and Hollomon 142 [24]. For certain alloys such as those of titanium, DRX is shown to contribute 143 significantly to the softening leading to the formation of ASB (see [25],[26])

144 2.1.1.2 Micro-voiding in the ASB wake

145 Although the ASBs occur in conditions of negative or nil stress triaxiality, micro-voids have been observed to form and grow within the bands. The micro-voiding could be 146 147 initiated in the band wake by the hydrostatic tension when there is a change in the 148 loading path. Or as stated in [20], when the loading is interrupted after the formation of 149 the ASB, the quenching of the hot band by the surrounding bulk material may lead to 150 phase transformation involving possible volume increase (as for martensitic 151 transformation) and strain incompatibility-induced crack formation at the band/matrix 152 interface. However, the ASB induced failure is generally observed under monotonic 153 loading.

Various perspectives on the stress triaxiality condition for the formation of micro-voids have been proposed which is discussed in section 3.1.1.3. Under a global shear pressure loading, Longère et al. [27] demonstrated that micro-voids can initiate and grow around inclusions in the material. Another theory cited by Odeshi et al. [11] is that the opening of the voids could be because of the high singular temperatures within the ASB causing

- atomic mobility or creating a lower flow stress in the ASB than the surrounding regularmaterial thereby generating a local tensile stress.
- 161 2.1.1.3 Ultimate rupture

The ASB by itself is not a failure mode i.e. a strong discontinuity but it acts as a precursor to premature material failure. The micro-voids which germinate within the ASB coalesce to the formation of cracks leading to the ultimate rupture of the material. Liu et al. [28] performed dynamic compression on Ti6Al4V alloy cylinders leading to ASB induced failure. The microscopic observation of the crushed specimens showed ASBs containing voids and coalesced voids (cracks).

168 **2.1.2 Mechanical consequences**

- 169 The mechanical consequences of ASB+MV initiation and evolution on the RVE (material
- 170 point) response are double: material and kinematic.
- 171 2.1.2.1 Preliminaries

ASBs are not a type of crack or a conventional 'damage' as there is cohesion of matter within the bands and without any surface separation. Neither are they slip bands which occur under quasi static conditions as the physics of the phenomenon is different. What is observed is a large gradient of the shear strain between the matrix and the band. It is considered here as a 'degradation' mechanism as it degrades the mechanical properties

177 of the overall material/structure in which it is present.

- ASBs are therefore classified as 'weak' discontinuity which involves a discontinuity of the gradient of the displacement/velocity i.e. of the strain/strain rate field. A 'strong' discontinuity such as a crack on the other hand involves a discontinuity of the displacement/velocity field. The weak discontinuity (ASB) serves as the path for the initiation of micro-voids which coalesce to form a strong discontinuity (crack) and the material fails. Like the ASB, the micro-voids formed in the wake of the ASB also have an effect on the deterioration and kinematic response of the material.
- In the present study, a large scale postulate is adopted, in which the representative volume element (RVE) has a length scale *W* greater than the ASB width λ , i.e. $W > \lambda$; in other words, the shear band is embedded within the RVE. In the presence of ASB coexist two different deformation patterns inside the medium: a 'regular' one relative to the material outside the bands, and a 'singular' one relative to the material inside the bands, see [21], [29]. Let suppose that the evolution of 'regular' and 'singular' processes can be

191 described via the evolution of state variables such like relevant measures of elastic 192 strain e^e , temperature *T*, strain hardening *k*; damage δ , metallurgical state ξ , and so on :

193
$$V_{\text{regular}} = \left(\mathbf{e}^{\mathbf{e}}, T, \kappa, \delta, \xi, \ldots\right) \text{ and } V_{\text{singular}} = \left(\mathbf{e}^{\mathbf{e}*}, T^*, \kappa^*, \delta^*, \xi^*, \ldots\right)$$

where V_{regular} and V_{singular} represent respectively the sets of 'regular' and 'singular' state
variables. At an advanced stage of deformation, 'singular' elastic strain can be neglected,
while a specific 'singular' variable describing intense shearing will be introduced
further. We then have tentatively:

198
$$V_{\text{regular}} = \left(\mathbf{e}^{\mathbf{e}}, T, \kappa, \delta, \xi, \ldots\right) \text{ and } V_{\text{singular}} = \left(T^*, \kappa^*, \delta^*, \xi^*, \ldots\right)$$

199 Before the ASB onset, solely 'regular' processes run:

200
$$V_{\text{regular}} = \left(\mathbf{e}^{\mathbf{e}}, T, \kappa, \delta, \xi, \ldots\right) \text{ and } V_{\text{singular}} = \left(0, 0, 0, 0, \ldots\right)$$

After the ASB onset, evolutions of 'regular' and 'singular' processes, associated to RVE whose length scale *W* is greater than the band width λ , i.e. *W*> λ , and which are respectively located outside and inside the band, become significantly distinct:

204
$$V_{\text{regular}} = (\mathbf{e}^{\mathbf{e}}, T, \kappa, \delta, \xi, ...) \text{ and } V_{\text{singular}} = (T^*, \kappa^*, \delta^*, \xi^*, ...)$$

In our approach, the evolution of the 'singular' dissipative processes (intervening inside the band) contributing to this macromechanical softening is described via the evolution of a single internal variable called \mathcal{D} . The softening of the RVE behaviour being considered as a form of mechanical degradation, the variable \mathcal{D} must then be able to describe the deterioration state of the RVE induced by the presence of the bands (ASB related feedback deterioration).

211 The variable \mathcal{D} is then a function of the 'singular' state variables and of the 212 characteristic length λ of the band:

213
$$\mathcal{D} = \mathcal{D}(V_{\text{singular}}) = \mathcal{D}(\lambda, T^*, \kappa^*, \delta^*, \xi^*, ...)$$

A micromechanical analysis followed by any averaging procedure could have lead to an explicit form for \mathcal{D} . This is not the purpose of the present work as it is hardly feasible regarding strongly non-linear phenomena involved and high strain rate context. What we are putting forward is a phenomenological description involving 'singular'

- dissipative evolution due to ASB and further micro-voiding entirely incorporated in the evolution of \mathcal{D} . In our phenomenological approach, evolution law of \mathcal{D} is derived from
- the normality rule under the assumption of the existence of a corresponding dissipative
- 221 potential.

222 2.1.2.2 Orientation

According to the large scale postulate, the shear band or the shear band cluster is considered as an entity embedded within the RVE, see Fig. 2. The vector **g** is collinear to the slip direction in the band plane and **n** represents the normal to the band plane. Accordingly, the structural tensors used in the following are defined in (1) where ()^S represents the symmetric and ()^{AS} the skew-symmetric parts of the tensor. According to experimental evidences, the ASBs develop along the planes of maximum shear stress within the RVE and thus their orientations are calculated.

230
$$\mathbf{N} = \mathbf{n} \otimes \mathbf{n} ; \mathbf{M} = (\mathbf{g} \otimes \mathbf{n})^{S} ; \mathbf{T} = (\mathbf{g} \otimes \mathbf{n})^{AS}$$
(1)



231 232 233

Fig. 2 ASB embedded within the RVE and orientation vectors

234 Different configurations of micro-voids developing in the ASB wake can be 235 distinguished. A thick wall cylinder implosion technique was carried out by Xue et al. [2] 236 to produce shear bands on Ti-6Al-4V alloys. The microscopic observation of the ASB 237 showed spherical void nucleation. The spherical voids were later seen to elongate to 238 ellipse shape rotate along the direction of the maximum shear stress. Impact tests on hat 239 shaped specimen by Peirs. et al. [1] showed micro-cracks in the wake of the ASB 240 oriented along the highly deformed grains which is different from the ASB orientation. 241 Accordingly, Fig. 3 shows an illustration of the possible micro-void shape and orientation vectors $\mathbf{n}^*, \mathbf{g}^*$ for micro-voiding occurring inside the band. Corresponding 242 243 MV structural tensors are denoted with an asterisk as N^*, M^*, T^* .



Fig. 3 Illustration of micro-void configurations. a) Spherical void configuration b) Ellipsoidal void
 configuration c) Micro-crack configuration.



As the ASB and MV are strongly oriented in space, they anisotropically degrade the elastic and plastic material properties of the RVE containing the band based on their orientation. The induced degradation may therefore be described by a 2nd order tensor variable **D** defined in (2). The components of **D** are: the scalar degradation intensities denoted by \mathcal{D}^{ASB} , \mathcal{D}^{MV} and the orientation tensors **N**,**N**^{*} of ASB and MV respectively.

$$D_{ij} = \mathcal{D}_{ASB} N_{ij} + \mathcal{D}_{MV} N_{ij}^*$$
(2)

253 Consider the illustration in Fig. 4, the normal to the ASB and to the MV is in direction 2,

in which case, the deterioration tensor is calculated below:





256

Fig. 4 Illustration ASB orientation normal to the 2 direction.

257
$$\mathbf{n} = \mathbf{n}^* = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \rightarrow \mathbf{N} = \mathbf{N}^* = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 \\ sym & 0 \end{bmatrix} \rightarrow \mathbf{D} = \left(\mathcal{D}^{ASB} + \mathcal{D}^{MV} \right) \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 \\ sym & 0 \end{bmatrix}$$
(3)

According to Fig. 4, the RVE can be viewed as a 3-layer material or sandwich material with a thin soft layer inserted between two thick hard layers, inducing a form of orthotropy. The resulting elastic shear modulus μ_{12} and elastic axial (Young's) modulus E_{22} are accordingly expected to progressively vanish while the other elastic moduli are not or less affected.

263
$$\begin{cases} \tau_{12} = 2\mu_{12}(\mathcal{D}_{ASB})e_{12}^{e} \\ \tau_{22} = E_{22}(\mathcal{D}_{ASB})e_{22}^{e} \end{cases} \text{ with } \begin{cases} \mu_{12}(\mathcal{D}_{ASB}) \rightarrow \mu_{c} \Box \mu_{0} \\ \mathcal{D}_{ASB} \rightarrow \mathcal{D}_{ASB} \rightarrow \mathcal{D}_{ASB} - \mathcal{D}_{ASB} \rightarrow \mathcal{D}_{ASB} - \mathcal{D}_{ASB} \rightarrow \mathcal{D}_{ASB} - \mathcal{D}_{ASB} - \mathcal{D}_{ASB} \rightarrow \mathcal{D}_{ASB} - \mathcal{D}_{ASB}$$

where τ is the elastic Kirchhoff stress tensor and \mathbf{e}^{e} the elastic strain tensor, (μ_{0}, E_{0}) and (μ_{c}, E_{c}) are the initial and critical, elastic shear and axial (Young's) moduli. Note that for the case of ASB, (μ_{c}, E_{c}) have non zero values since ASB preserves matter cohesion.

Furthermore, the effect of the combined deterioration of ASB and MV can be seen on the strain hardening force $r(\kappa)$ as presented in Fig. 5. The black curve represents the strain hardening solely as a function of the isotropic hardening variable κ . The blue curve carries an additional influence of the temperature i.e. thermal softening. The purple curve is subjected to the ASB and MV induced deterioration and hence the reduction in hardening or conversely softening behaviour.

274 2.1.2.4 Kinematic consequences

The kinematic consequences of the presence of the ASB and hence MV are viewed asthose of a 'macro-dislocation' considering an RVE as illustrated in Fig. 6.

277







279

280Fig. 6 ASB viewed as a macro dislocation and the equivalent RVE with kinematic consequences. The281kinematic variables L^{ASB} and L^{MV} allow to smooth the boundary discontinuity caused by the ASB and282MV, as in crystalline plasticity and continuum damage mechanics.

283 We are designating the total velocity gradient \mathbf{L} as the sum of a symmetric part \mathbf{d} , the and antisymmetric 284 strain rate, an part ω, the spin rate, i.e. $\mathbf{L} = \mathbf{d} + \boldsymbol{\omega}$; $\mathbf{d} = \text{sym}[\mathbf{L}]$; $\boldsymbol{\omega} = \text{antisym}[\mathbf{L}]$. The velocity gradient created by the regular 285 plastic deformation outside the band is designated as \mathbf{L}^{p} . The ASB induces a 286 supplementary velocity gradient \mathbf{L}^{ASB} as a result of glide velocity $\dot{\gamma}^{ASB}$ in the direction of 287 the unit vector ${\bf g}$; likewise the MV induced velocity gradient is termed as ${\bf L}^{^{MV}}.$ The 288 introduction of \mathbf{L}^{ASB} and \mathbf{L}^{MV} facilitates the smoothening of the boundary discontinuity 289 caused by ASB as it is done in crystalline plasticity, see Fig. 6. 290

291
$$\mathbf{L}^{in} = \mathbf{L}^{p} + \mathbf{L}^{ASB} + \mathbf{L}^{MV}$$
(5)

292 The deterioration-induced velocity gradient for a given band pattern α is partitioned 293 into symmetric and skew-symmetric parts leading to the corresponding strain rate **d** 294 and spin ω respectively as given below.

295
$$L_{ij}^{ASB} \propto \sum_{\alpha} \dot{\gamma}^{ASB,\alpha} g_{i}^{\alpha} n_{j}^{\alpha} \begin{cases} d_{ij}^{ASB} \propto \sum_{\alpha} \dot{\gamma}^{ASB,\alpha} M_{ij}^{\alpha} \\ \omega_{ij}^{ASB} \propto \sum_{\alpha} \dot{\gamma}^{ASB,\alpha} T_{ij}^{\alpha} \end{cases}$$
$$\left\{ d_{ij}^{MV} \propto \sum_{\alpha} \dot{\gamma}^{ASB,\alpha} M_{ij}^{\alpha} + \frac{\dot{\varepsilon}_{m}^{MV}}{3} I_{ij} \begin{cases} d_{ij}^{MV} \propto \sum_{\alpha} \dot{\gamma}^{MV,\alpha} M_{ij}^{*\alpha} + \frac{\dot{\varepsilon}_{m}^{MV}}{3} I_{ij} \\ \omega_{ij}^{MV} \propto \sum_{\alpha} \dot{\gamma}^{MV,\alpha} T_{ij}^{*\alpha} \end{cases} \right\}$$
(6)

In case of MV configurations accounting for the void expansion, an additional hydrostatic term appears in the strain rate, where **I** is the identity tensor and $\dot{\varepsilon}_m^{MV}$ is the mean strain rate.

The kinematic consequences of the presence of ASB and MV are thus shown by the total inelastic strain rate \mathbf{d}^{in} resulting from the superposition of regular plastic strain rate $\mathbf{d}^{in(PP)}$ by the singular strain rates $\mathbf{d}^{in(ASB)}$ and $\mathbf{d}^{in(MV)}$.

302
$$d_{ij}^{in} = d_{ij}^{in(PP)} + d_{ij}^{in(ASB)} + d_{ij}^{in(MV)}$$
(7)

303 A schematic representation of the kinematics is shown in Fig. 7 where F in all the three 304 cases represents the plastic potential in absence of the deterioration mechanisms. Fig. 305 7a shows the case of regular plasticity before the appearance of ASB during which the total inelastic strain rate reduces to $\mathbf{d}^{in} = \mathbf{d}^{in(PP)} = \Gamma^{PP} \mathbf{m}$ where Γ^{PP} is the regular plastic 306 yield intensity and $\mathbf{m}=(3/2)\mathbf{x}(\mathbf{s}/\sigma_{eq})$ the yield direction (normality rule) with σ_{eq} 307 308 designating Mises equivalent stress and s the deviatoric part of the Kirchhoff stress The ASB formation in Fig. 7b superposes an additional strain rate 309 tensor. $\mathbf{d}^{\textit{in}(\textit{ASB})} = \Gamma^{\textit{ASB}} \mathbf{M}$, causing progressive deviation of the yield direction and loss of 310 coaxiality between inelastic strain rate and stress deviator (general case). Finally, the 311 312 micro-voiding in Fig. 7c further contributes to the yield intensity Γ^{MV} (assuming 313 collinearity of ASB and MV orientations, see Fig. 4) and keeps on deviating the yield 314 direction, provoking in particular a plastic expansion termed as MV_{hydrostatic}.

- For the different possible configurations of MV in Fig. 3, the following lists the MV induced effects:
- a) The first simple configuration assumes ideal spherical voids in Fig. 3a. In this case, the spherical MV contributes to isotropic degradation $(Tr\dot{\mathbf{D}})$ and hydrostatic plastic strain rate (\mathbf{d}_{ν}^{p}) accounting for volume change only.

b) Then the second configuration considered shows elliptical voids which possess an orientation $(\mathbf{n}^*, \mathbf{g}^*)$ which may or may not be the same as that of the ASB (Fig. 3b). These types of elliptical voids contribute to anisotropic degradation rate ($\dot{\mathbf{D}} = \dot{\mathcal{D}}_{MV} \mathbf{N}^*$; $\mathbf{N}^* = \mathbf{n}^* \otimes \mathbf{n}^*$) and hydrostatic and deviatoric (\mathbf{d}_s^p) strain rates (with the corresponding tensor $\mathbf{M}^* = (\mathbf{g}^* \otimes \mathbf{n}^*)^S$) accounting for volume and shape changes respectively.

326 c) The third configuration in Fig. 3c presents micro-cracks with orientation $\mathbf{n}^*, \mathbf{g}^*$ 327 and which influence the anisotropic degradation rate $(\dot{\mathcal{D}}_{_{MV}}, \mathbf{N}^*)$ only. When 328 crack opening is not taken into account, there is no MV related strain rate.



Fig. 7 Illustration of yield direction evolution (a) before ASB onset (b) during adiabatic shear banding (c)
 during micro-voiding. F is the regular plastic potential in the absence of deterioration mechanisms.

331 2.2 CONSTITUTIVE MODELLING

332 This section deals with the more specific form of the unified constitutive model 333 describing the ASB and the consequent MV induced deterioration. The 334 phenomenological model describing ASB induced failure originally developed by 335 Longère et al [21] has been conceptually improved by Longère and Dragon [22] to 336 incorporate the effects of micro-voiding (MV) in the post critical stage. The model used 337 in the present work is mostly based on the enlarged model in [22] while making some 338 simplifications/modifications. The role of dynamic recrystallization on the onset of ASB 339 in the materials susceptible to this mechanism has also been considered here. The aim of 340 the ASB+MV model is to clearly distinguish the contributions to the degradation coming 341 from the ASB on the one hand and the MV on the other hand. The constitutive model 342 presenting the dynamic recrystallization in the context of the model under consideration 343 can be found in [30].

The constitutive model developed here is a phenomenological one wherein the consequences of the presence of the ASB at the global RVE scale on the regular properties are described. The salient physical features described by the model are:

- 347 • softening influencing ASB onset: plastic dissipation induced thermal softening 348 • 349 • dynamic recrystallization (DRX) induced softening 350 consequences: ٠ 351 • anisotropic material deterioration due to ASB+MV
- 352
 - ASB+MV induced specific finite strain kinematics

353 In the following, the quantities/properties associated with the material inside the ASB 354 are termed as 'singular' and the quantities/properties associated with the material 355 outside the band are referred to as 'regular'.

2.2.1 Large anisotropic strain framework 356

As very large strains and rotations are encountered during the ASB process, a finite 357 elastic-plastic deformation framework assuming moderate elastic deformation is 358 adopted. The objective corotational derivative $\overset{\vee}{\mathbf{A}}$ of a 2nd order tensor \mathbf{A} is given by 359

$$360 \qquad \mathbf{\dot{A}} = \mathbf{\dot{A}} - \mathbf{W}\mathbf{A} + \mathbf{A}\mathbf{W}$$
(8)

361 where **W** represents the rotation rate of anisotropy axes relative to ASB orientation. 362 Taking into account the negligible elastic rotation ω^e and relative small regular plastic spin $\omega^{in(PP)}$, see [21], the rotation rate **W** is reduced to: 363

364
$$\mathbf{W} = \boldsymbol{\omega} \cdot \left(\boldsymbol{\omega}^{in(ASB)} + \boldsymbol{\omega}^{in(MV)}\right)$$
(9)

where $\omega^{in(ASB)}$ and $\omega^{in(MV)}$ are the spin rates induced by ASB and MV respectively. In the 365 366 following, the tensors **X** defined in the intermediate configuration are transported to the current one denoted by a tilde $\tilde{\mathbf{X}}$ via $\tilde{\mathbf{X}} = \mathbf{O}\mathbf{X}\mathbf{O}^{\mathrm{T}}$, $\mathbf{W} = \dot{\mathbf{O}}\mathbf{O}^{\mathrm{T}}$. 367

2.2.2 Thermodynamic framework 368

369 In the framework of irreversible thermodynamics, the (regular) state variables to account for are: the elastic strain tensor $e^e = \ln V^e$, the absolute temperature T, the 370 isotropic hardening variable κ . The singular temperature and other singular state 371 372 variables are not explicitly calculated in the model, but their effects on the material 373 degradation are embodied in the degradation tensor $\tilde{\mathbf{D}}$.

Helmholtz free energy $\psi(\mathbf{e}^{e}, T, \kappa; \tilde{\mathbf{D}})$ is assumed as the state potential comprising of a reversible part $\psi^{e}(\mathbf{e}^{e}, T; \tilde{\mathbf{D}})$, a stored energy part $\psi^{p}(T, \kappa; \tilde{\mathbf{D}})$ and a purely thermal part $\psi^{T}(T)$ as shown in (10). The presence of ASB affects both the elastic and plastic properties.

378
$$\psi(\mathbf{e}^{e}, T, \kappa; \tilde{\mathbf{D}}) = \psi^{e}(\mathbf{e}^{e}, T; \tilde{\mathbf{D}}) + \psi^{p}(T, \kappa; \tilde{\mathbf{D}}) + \psi^{T}(T)$$
 (10)

Constitutive state laws derived from the state potential in (10) allows for expressing the elastic Kirchhoff stress tensor τ , strain hardening force r, deterioration driving force \tilde{G} and entropy s, as follows:

$$\tau_{ij} = \rho_0 \frac{\partial \psi}{\partial e_{ij}^e} = \rho_0 \frac{\partial \psi^e}{\partial e_{ij}^e} ; r = \rho_0 \frac{\partial \psi}{\partial \kappa} = \rho_0 \frac{\partial \psi^p}{\partial \kappa}$$

$$382 \qquad \tilde{G}_{ij} = -\rho_0 \frac{\partial \psi}{\partial \tilde{D}_{ij}} = -\left(\rho_0 \frac{\partial \psi^e}{\partial \tilde{D}_{ij}} + \rho_0 \frac{\partial \psi^p}{\partial \tilde{D}_{ij}}\right)$$

$$\rho_0 s = -\rho_0 \frac{\partial \psi}{\partial T} = -\left(\rho_0 \frac{\partial \psi^e}{\partial T} + \rho_0 \frac{\partial \psi^p}{\partial T} + \rho_0 \frac{\partial \psi^T}{\partial T}\right)$$

$$(11)$$

383 where ρ_0 designates the initial mass density. The model should satisfy the Clausius-384 Duhem inequality in order to be consistent with the irreversible thermodynamics. 385 Therefore the intrinsic dissipation \mathfrak{D}_{int} is expressed as:

386
$$\mathfrak{D}_{int} = \tau_{ij}d_{ji} - \rho_0(\dot{\psi} + sT) \ge 0$$
(12)

387 \mathfrak{D}_{int} is decomposed into regular plasticity related term \mathfrak{D}_{reg} and singular ASB+MV 388 induced term \mathfrak{D}_{sing} . Using the Gibbs relation $\rho_0 \dot{\psi} = \tau_{ij} d_{ij}^e + r \dot{\kappa} - \tilde{G}_{ij} \dot{\tilde{D}}_{ij} - \rho_0 s \dot{T}$ the 389 dissipation components are written as:

$$\mathfrak{D}_{int} = \mathfrak{D}_{reg} + \mathfrak{D}_{sing} \ge 0
\mathfrak{D}_{reg} = \tau_{ij} d_{ji}^{p} - r \dot{\kappa} \ge 0 ; \ \mathfrak{D}_{sing} = \tau_{ij} d_{ji}^{d} + \tilde{G}_{ij} \tilde{D}_{ji} \ge 0 ; \begin{cases} d_{ij}^{p} = d_{ij}^{in(PP)} \\ d_{ij}^{d} = d_{ij}^{in(ASB)} + d_{ij}^{in(MV)} \end{cases}$$
(13)

In the context of generalised normality rule, the evolutions laws are correspondingly derived from dissipation potentials namely the viscoplastic potential ϕ_p and viscousdegradation potential $\phi_d = \phi_{ASB} + \phi_{MV}$ as:

$$d_{ij}^{in} = \frac{\partial \phi_p}{\partial \tau_{ij}} = d_{ij}^{in(PP)} + d_{ij}^{in(ASB)} + d_{ij}^{in(MV)}$$

$$-\dot{\kappa} = \frac{\partial \phi_p}{\partial r}$$

$$\tilde{D}_{ij} = \frac{\partial \phi_d}{\partial G_{ij}} = \tilde{D}_{ij}^{\Lambda SB} + \tilde{D}_{ij}^{MV}$$

(14)

394

395 It is now required to define a plastic potential H and/or a yield function F depending 396 on whether non-associated ($H \neq F$) or associated flow rule (H = F) is followed.

397 **2.2.3 Constitutive equations**

A more precise form of the constitutive equations adopted in the current study is presented in this section. In the following, for simplification, elliptical void shape is assumed with the orientation along the direction of the ASB as represented in Fig. 8. Hence the structural tensors in (1) corresponding to the ASB and MV are considered to be the same (**N**, **M**).



403

404

Fig. 8 Elongated micro-voids oriented in the direction of ASB

405 2.2.3.1 Preliminary considerations

406 • Elastic stress tensor

Following the work of Halm and Dragon [31], see also Longère and Dragon [21], the
elastic stress tensor in presence of anisotropic damage induced degradation is assumed
of the form:

account material

412 The form given to the stress tensor in (15) is such that it takes into account material
413 degradation based on the orientation of the shear bands.
$$\lambda$$
 and μ represent the Lamé
414 elasticity constants and $K = (3\lambda + 2\mu)/3$ the bulk modulus. *a* and *b* are ASB+MV related
415 constants inducing orthotropic elastic energy degradation – they may have different
416 values for ASB and MV in a future work. In the thermal part, $\bar{\alpha}$ represents the thermal

- expansion coefficient, T_0 the initial temperature and $\Delta T = T T_0$ the rise in temperature. 417
- 418 Consider now the illustration in Fig. 4, the normal to the ASB is in direction 2, in which case, the deterioration tensor is calculated below: 419

420
$$\mathbf{n} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \rightarrow \mathbf{D} = \mathcal{D} \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 \\ sym & 0 \end{bmatrix}; \ \mathcal{D} = \mathcal{D}^{ASB} + \mathcal{D}^{MV}$$
(16)

421 By neglecting the thermal dilatation, the components of τ for the above case (Fig. 4) 422 deduced from (15)-(16) are:

423
$$\begin{cases} \tau_{11} = (\lambda + 2\mu)e_{11}^{e} + (\lambda - a\tilde{D}_{22})e_{22}^{e} + \lambda e_{33}^{e} \\ \tau_{22} = (\lambda - a\tilde{D}_{22})(e_{11}^{e} + e_{33}^{e}) + [(\lambda - 2a\tilde{D}_{22}) + 2(\mu - 2b\tilde{D}_{22})]e_{22}^{e} \\ \tau_{33} = (\lambda + 2\mu)e_{33}^{e} + (\lambda - a\tilde{D}_{22})e_{22}^{e} + \lambda e_{11}^{e} \end{cases}$$
(17)

424
$$\begin{cases} \tau_{12} = 2(\mu - b\tilde{D}_{22})e_{12}^{e} \\ \tau_{13} = 2\mu e_{13}^{e} \\ \tau_{23} = 2(\mu - b\tilde{D}_{22})e_{23}^{e} \end{cases}$$

The resulting (symmetric) stiffness matrix \mathbf{C} , $\mathbf{\tau} = \mathbf{C} : \mathbf{e}^{e}$, reads 425

$$426 \quad [C] = \begin{bmatrix} \lambda + 2\mu & (\lambda - aD) & \lambda & 0 & 0 & 0 \\ & (\lambda - 2aD) + 2(\mu - 2bD) & (\lambda - aD) & 0 & 0 & 0 \\ & & \lambda + 2\mu & 0 & 0 & 0 \\ & & & 2(\mu - bD) & 0 & 0 \\ & & & & & 2(\mu - bD) \end{bmatrix}$$
(18)

427 Failure under shear loading yields an upper bound for deterioration intensity \mathcal{D}_c as shown 428 below:

429
$$\tau_{12} = 2(\mu - b\mathcal{D}_c)e_{12}^e = 0 \quad \rightarrow \quad \mathcal{D}_c = \frac{\mu}{b} \rightarrow \mathcal{D}_c(b = \mu) = 1 \tag{19}$$

430 A reduction in the material strength is seen in the direction normal to the ASB (τ_{22}) and 431 in the corresponding shear direction (τ_{12}). It is seen that the constants a < 0 and b > 0432 contribute to the reduction in Young's modulus E_{22} whereas only b acts in the 433 reduction of the shear modulus μ_{12} .

• Strain hardening force

Experimental observations have shown that in absence of ASB and MV the coupling
between strain hardening and thermal softening may be described in a product form
allowing for using the method of separation of variables

438
$$r(\kappa,T) = \rho_0 \frac{\partial \psi}{\partial \kappa} = \rho_0 \frac{\partial \psi^p}{\partial \kappa} = h'(\kappa) g(T)$$
(20)

439 The form of the thermal softening corresponding to steel is shown in (21) where v is the 440 material specific thermal softening constant

441
$$g(T) = \exp(-\upsilon T)$$
(21)

For materials such as titanium alloys, in accordance with experimental observations, the function in (22) satisfies the thermal softening characteristics with T_{ref} being a reference temperature such that $g(T_{ref}) = 0$. $\langle . \rangle$ are Macauley brackets defined as $\langle x \rangle = \max(x, 0)$.

445
$$g(T) = \left\langle 1 - \left(\frac{T}{T_{ref}}\right)^t \right\rangle$$
(22)

446 where *t* designates a constant. The strain hardening function is expressed in (23) where 447 R_{∞} is related to the saturation of isotropic hardening (Voce law).

448
$$h'(\kappa) = R_{\infty} \left[1 - \exp(-k\kappa) \right]; h(\kappa) = R_{\infty} \left[\kappa + \frac{1}{k} \exp(-k\kappa) \right]$$
(23)

449 We are here assuming that this product form can be extended for ASB and MV

450
$$r(\kappa, T; \tilde{\mathbf{D}}) = \rho_0 \frac{\partial \psi}{\partial \kappa} = \rho_0 \frac{\partial \psi^p}{\partial \kappa} = h'(\kappa) g(T) w(\tilde{\mathbf{D}})$$
(24)

In the following equations the thermal softening function in (21) is used. The deterioration function $w(\tilde{\mathbf{D}})$ is expressed below where χ_1 and χ_2 are ASB+MV related deterioration constants. The form of the deterioration function $w(\tilde{\mathbf{D}})$ is adopted of the same exponential form as the thermal softening function in (21) as the singular temperature rise within the shear band is the main contributor to the material deterioration. The expression of $w(\tilde{\mathbf{D}})$ in (25) is tentatively retained for other materials such as Ti alloys even though the form of their thermal softening function is different.

458
$$w(D_{ij}) = \exp\left(-\chi_1 \tilde{D}_{ii} - \frac{\chi_2}{2} \tilde{D}_{ij} \tilde{D}_{ji}\right)$$
(25)

459 2.2.3.2 State potential

According to the preliminary considerations above, the state potential reads after integration of the constitutive state laws in (15) and (24) with respect to their different arguments:

463
$$\psi(\mathbf{e}^{e}, T, \kappa; \tilde{\mathbf{D}}) = \psi^{e}(\mathbf{e}^{e}, T; \tilde{\mathbf{D}}) + \psi^{p}(T, \kappa; \tilde{\mathbf{D}}) + \psi^{T}(T)$$

$$\begin{cases} \rho_{0}\psi^{e}(\mathbf{e}^{e}, T; \tilde{\mathbf{D}}) = \frac{1}{2}\mathbf{e}^{e} : \mathbf{C}(\tilde{\mathbf{D}}) : \mathbf{e}^{e} - \overline{\alpha}K.Tr(\mathbf{e}^{e}).\Delta T \\ \rho_{0}\psi^{p}(T, \kappa; \tilde{\mathbf{D}}) = h(\kappa)g(T)w(\tilde{\mathbf{D}}) \\ \rho_{0}\psi^{T}(T) = -\rho_{0}\frac{C}{2T_{0}}\Delta T^{2} \end{cases}$$
(26)

465 where *C* designates the specific heat.

466 2.2.3.3 Constitutive state laws

The complete expressions of the conjugate forces associated to the state variables,considering steel oriented thermal softening function, is shown below:

$$469 \qquad \begin{cases} \tau_{ij} = \lambda e_{kk}^{e} I_{ij} + 2\mu e_{ij}^{e} - \overline{\alpha} K \Delta T I_{ij} - a \left(e_{mn}^{e} \tilde{D}_{nm} I_{ij} + e_{kk}^{e} \tilde{D}_{ij} \right) - 2b \left(e_{ik}^{e} \tilde{D}_{kj} + \tilde{D}_{ik} e_{kj}^{e} \right) \\ r = R_{\infty} \left[1 - \exp\left(-k\kappa \right) \right] \exp\left(-\nu T \right) \exp\left(-\chi_{1} \tilde{D}_{kk} - \frac{\chi_{2}}{2} \tilde{D}_{kl} \tilde{D}_{lk} \right) \\ \tilde{G}_{ij} = a e_{kk}^{e} e_{ij}^{e} + 2b e_{ik}^{e} e_{kj}^{e} + R_{\infty} \left[\kappa + \frac{1}{k} \exp\left(-k\kappa \right) \right] \\ \cdot \exp\left(-\nu T \right) \exp\left(-\chi_{1} \tilde{D}_{kk} - \frac{\chi_{2}}{2} \tilde{D}_{kl} \tilde{D}_{lk} \right) \left[\chi_{1} I_{ij} + \chi_{2} \tilde{D}_{ij} \right] \end{cases}$$

$$(27)$$

470 The expression of the entropy is not detailed here. The diminution of the stress τ is 471 caused by the isotropic heating and ASB+MV induced anisotropic degradation. The 472 competition between hardening and softening is embodied in the isotropic hardening 473 conjugate force r: the strain hardening capability $\partial r / \partial \kappa$ is decreased by the thermal 474 softening function g(T). In addition, as the deterioration **D** evolves, the deterioration 475 related function $w(\tilde{\mathbf{D}})$ magnifies the loss of the strain hardening capability as illustrated 476 in Fig. 5. In isothermal conditions and in the absence of deterioration, r reaches a saturation stress $R_{\infty} \exp(-\upsilon T_0)$ relative to isotropic hardening. The deterioration 477 conjugate force $\tilde{\mathbf{G}}$ has contributions from the reversible part ψ^{e} and stored energy part 478 ψ^{p} of the free energy which correspondingly represent the elastic and stored energy 479 release rate. $ilde{\mathbf{G}}$ in the following is contained in $\Delta G_{\scriptscriptstyle ASB}$ and $\Delta G_{\scriptscriptstyle MV}$ through the scalar 480 quantity G obtained by the projection of $ilde{\mathbf{G}}$ onto the band plane. In particular, the values 481 of G at the ASB and MV onset are considered namely G_{ASB} and G_{MV} respectively and the 482 483 quantities ΔG_{ASB} and ΔG_{MV} which are defined as:

484
$$G = \tilde{G}_{ij} N_{ji} ; \Delta G_{ASB} = \langle G - G_{ASB} \rangle ; \Delta G_{MV} = \langle G - G_{MV} \rangle$$
(28)

485 It is to be noted that the deterioration conjugate force exists and evolves even before the 486 deterioration onset. A finite supply of local energy release rate (G_{ASB} , G_{MV}) is required to 487 activate the deterioration (ASB, MV). The deterioration onset criteria and calculation of 488 G_{ASB} and G_{MV} are defined in section 2.3.

489 2.2.3.4 Yield function

490 Various void induced damage models exist in the literature. Lemaitre [32] modelled 491 ductile damage considering non-dilatant effect of void growth. The dilatant void growth 492 models of Rousselier [33] and GTN (Gurson-Tvergaard-Needleman) ([34],[35]) are 493 widely used damage plasticity models to describe ductile damage. The ASB induced 494 degradation, in the present study, was initially described using a thermo/elastic-495 viscoplastic-deterioration (TEVPD) model. Now, in order to describe the post critical 496 micro-voiding, rather than using another plasticity-ductile damage coupled model, a 497 'unified approach' is adopted wherein the MV induced consequences are merged within 498 the TEVPD framework without distorting much its formal structure. The unified 499 enlarged model has some analogies with Rousselier model [33] for its dependence on hydrostatic stress via an exponential function that notably allows for reproducing void 500 501 growth under shear loading.

502 The yield function F_{total} when both the ASB and MV mechanisms are in operation reads:

503
$$\mathbf{F}_{total} = \sigma_{eq} + 3\xi \Delta G_{MV}^2 \exp\left(\frac{\sigma_m}{\overline{\sigma}}\right) - (R_0 + r) = \sigma_v \ge 0$$
(29)

where σ_{eq} is the transformed equivalent stress accounting for the anisotropy induced in the plastic flow by evolving ASB and MV, $(R_0 + r)$ the rate independent yield stress with r the strain hardening force, σ_v the strain rate induced overstress, $\sigma_m = \tau_{kk} / 3$ the mean stress and $\bar{\sigma}$ a reference stress. R_0 is expressed in (30) with R_{int} being the internal stress (thermal softening function related to steel).

509
$$R_0 = R_{int} \exp(-\upsilon T) \exp\left(-\chi_1 \tilde{D}_{kk} - \frac{\chi_2}{2} \tilde{D}_{kl} \tilde{D}_{lk}\right)$$
(30)

510 The second term of the expression of F_{total} containing σ_m corresponds to the expansion of 511 micro-voids with ξ being the related material constant. The ΔG_{MV} in this term has been 512 modified to ΔG_{MV}^2 from the previous work ([22],[36],[37]) in order to be consistent with 513 the MV incipience while deriving the deterioration rate expressed in (39)₂ below.

514 2.2.3.5 Equivalent stress

515 As mentioned above, a transformed equivalent stress σ_{eq} is used here which 516 incorporates the regular plasticity and the anisotropy induced in the plastic flow 517 provoked by the formation (onset and evolution) of the strongly oriented deterioration 518 mechanisms at stake (ASB+MV) through a 4th order tensor **P** as shown below:

519
$$\sigma_{eq} = \sqrt{\frac{3}{2}} \mathbf{s} \cdot \mathbf{P} (\Delta G_{ASB}, \Delta G_{MV}) \cdot \mathbf{s} ; \mathbf{P} = \mathbf{I} + 2 (\eta_{ASB} \Delta G_{ASB}^2 + \eta_{MV} \Delta G_{MV}^2) \mathbf{M} \otimes \mathbf{M}$$
(31)

520 where **s** is the deviatoric part of the Kirchhoff stress tensor, **I** the 4th order identity 521 tensor, $I_{ijkl} = \frac{1}{2} \left(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right)$, and η_{ASB} and η_{MV} material constants relative to the 522 corresponding mechanisms. A power of 2 is used for ΔG_{ASB} and ΔG_{MV} terms, see their 523 definitions in (28), in the above expression in order to ensure the concomitance of the 524 deterioration induced rates while deriving their expressions later in (37) and (39) 525 below. The transformed equivalent stress σ_{eq} in (31) may also be expressed of the form:

526
$$\sigma_{eq} \equiv \sqrt{\sigma_{VM}^{2} + \sigma_{ASB}^{2} + \sigma_{MV}^{2}}; \begin{cases} \sigma_{VM} = \sqrt{\frac{3}{2}} \mathbf{s} \cdot \mathbf{s} \\ \sigma_{ASB} = \sqrt{3} \eta_{ASB} \Delta G_{ASB} \tau_{res} \\ \sigma_{MV} = \sqrt{3} \eta_{MV} \Delta G_{MV} \tau_{res} \end{cases}$$
(32)

527 where $\tau_{res} = |\mathbf{s}: \mathbf{M}|$ represents the shear stress resolved along the band plane. σ_{eq} in (32) 528 therefore has contributions from the regular and singular mechanisms and is composed 529 of the regular plastic von Mises equivalent stress σ_{VM} and the singular stresses induced 530 by ASB - σ_{ASB} and then by MV- σ_{MV} .

531 One can note that, in the absence of MV ($\Delta G_{MV} = 0$), F_{total} in (29) reduces to F_{PP+ASB} i.e. 532 yield function in the presence of ASB only. Further in the absence of ASB ($\Delta G_{ASB} = 0$), 533 Von Mises yield criterion F_{PP} is followed. The different possible cases of the yield 534 function in the presence or absence of ASB and MV are shown in Table 1.

The expressions for the singular contributions to the equivalent stress are modified here from the earlier versions in order to take into account the loss of strength of the material due to ASB and the subsequent MV in the direction normal to the band during tension loading by adding the stress term $\sigma_N = \langle \tau : \mathbf{N} \rangle = \max(0, \tau : \mathbf{N})$ in the expression of the transformed equivalent stress:

$$\hat{\sigma}_{eq} \equiv \sqrt{\sigma_{VM}^{2} + \hat{\sigma}_{ASB}^{2} + \hat{\sigma}_{MV}^{2}}; \begin{cases} \hat{\sigma}_{ASB} \equiv \sqrt{\eta_{ASB} \left(3\tau_{res}^{2} + \alpha \sigma_{N}^{2} \right)} \Delta G_{ASB} \\ \hat{\sigma}_{MV} \equiv \sqrt{\eta_{MV} \left(3\tau_{res}^{2} + \alpha \sigma_{N}^{2} \right)} \Delta G_{MV} \end{cases}$$
(33)
$$\mathbf{F}_{total} = \hat{\sigma}_{eq} \left(\mathbf{s}, \Delta G_{ASB}, \Delta G_{MV} \right) + 3\xi \Delta G_{MV}^{2} \exp \left(\frac{\sigma_{m}}{\overline{\sigma}} \right) - \left(R_{0} + r \right) = \sigma_{v} \ge 0$$

Table 1 Form of yield function in the presence or absence of ASB and MV

540

| Operating Mechanisms | ΔG | $\sigma_{_{eq}}{}^{2}$ | $\mathbf{F} = \boldsymbol{\sigma}_{v} \ge 0$ |
|-------------------------|--|--|--|
| PP + ASB + MV | $\Delta G_{ASB} \neq 0$ $\Delta G_{MV} \neq 0$ | $\sigma_{VM}^{2} + \sigma_{ASB}^{2} + \sigma_{MV}^{2}$ | $F_{total} = \sigma_{eq} \left(\mathbf{s}, \Delta G_{ASB}, \Delta G_{MV} \right) + 3 \xi \Delta G_{MV}^2 \exp \left(\frac{\sigma_m}{\overline{\sigma}} \right) - \left(R_0 + r \right)$ |
| PP + ASB | $\Delta G_{ASB} \neq 0$ $\Delta G_{MV} = 0$ | $\sigma_{_{V\!M}}{}^2 + \sigma_{_{ASB}}{}^2$ | $\mathbf{F}_{PP+ASB} = \boldsymbol{\sigma}_{eq} \left(\mathbf{s}, \Delta G_{ASB}, 0 \right) - \left(R_0 + r \right)$ |
| PP | $\Delta G_{ASB} = 0$ $\Delta G_{MV} = 0$ | $\sigma_{_{V\!M}}{}^2$ | $\mathbf{F}_{PP} = \boldsymbol{\sigma}_{eq} \left(\mathbf{s}, 0, 0 \right) - \left(R_0 + r \right)$ |

542 The value of the coefficient α is assigned 3 in the present work. The scalar function 543 preceding $\mathbf{M} \otimes \mathbf{M}$ in the original expression of **P** (see equation (36) in [22]) has been limited here to a single term. In a certain way, the a posteriori addition of $\sigma_{\scriptscriptstyle N}$ in the 544 545 transformed equivalent stress allows for palliating the aforementioned truncation. 546 During tension loading in the direction normal to the shear band, presumably the entire load is carried by the shear bands. During normal compression loading, when $\tau_{\rm res}=0$ 547 and $\sigma_{_N} = 0$, the RVE is supposed to contain no shear bands and the entire load is carried 548 549 by the regular matrix material.

It is to be remarked that ASB induced deterioration is in operation during the loading duration when the shear band is still soft. With longer duration or during interrupted loading, the material within the ASB would possibly undergo phase transformation due to quenching by the surrounding regular material and become harder. In this case, the material regains its near original strength except for the irreversible MV deterioration. This remark is to be taken into account in the prospective work.

556 2.2.3.6 Viscoplastic and viscous-damage potential

557 The existence of viscoplastic potential ϕ_p and viscous-deterioration potential ϕ_{ASB} , ϕ_{MV}

of Norton-Perzyna's type is assumed in the form of power law:

559
$$\phi_p = \frac{Y}{n+1} \left\langle \frac{H}{Y} \right\rangle^{n+1}; \quad \phi_{ASB} = \frac{Z}{m+1} \left\langle \frac{H}{Z} \right\rangle^{m+1}; \quad \phi_{MV} = \frac{W}{q+1} \left\langle \frac{H}{W} \right\rangle^{q+1}$$
(34)

560 *Y* and *n* are viscous constants corresponding to the regular plasticity; *Z*, *m* and *W*, *q* 561 are time-dependence related constants corresponding to the ASB and MV degradation 562 mechanisms respectively.

563 2.2.3.7 Evolution laws

A non-associated plasticity is followed such that the plastic potential $H = F_{total} (\sigma_N \equiv 0)$ as expressed below.

566
$$H = \sigma_{eq} + 3\xi \Delta G_{MV}^2 \exp\left(\frac{\sigma_m}{\overline{\sigma}}\right) - (R_0 + r)$$
(35)

567 The viscoplastic multiplier Λ_p and viscous-deterioration multipliers Λ_{ASB} , Λ_{MV} are 568 expressed below.

569
$$\Lambda_{p} = \left\langle \frac{\partial \phi_{p}}{\partial F} \right\rangle = \left\langle \frac{H}{Y} \right\rangle^{n}; \quad \Lambda_{ASB} = \left\langle \frac{\partial \phi_{d}}{\partial F} \right\rangle = \left\langle \frac{H}{Z} \right\rangle^{m}; \quad \Lambda_{MV} = \left\langle \frac{\partial \phi_{d}}{\partial F} \right\rangle = \left\langle \frac{H}{W} \right\rangle^{q}$$
(36)

570 The detailed rate equations derived from the plastic potential according to the normality 571 rule are shown below. In addition to the deviatoric component, the MV induced strain 572 rate $\mathbf{d}^{in(MV)}$ is also composed of a hydrostatic component. The MV expansion described 573 by the dependence on the mean stress according to $\exp(\sigma_m / \overline{\sigma})$ was initially proposed by 574 Rice and Tracey [38].

575

$$\begin{cases} d_{ij}^{in(PP)} = \frac{3}{2} \Lambda_P \frac{s_{ij}}{\sigma_{eq}} \\ d_{ij}^{in(ASB)} = 3\Lambda_P \frac{\eta_{ASB} \Delta G_{ASB}^2 \tau_{res}}{\sigma_{eq}} M_{ij} \\ d_{ij}^{in(MV)} = 3\Lambda_P \left[\frac{\eta_{MV} \Delta G_{MV}^2 \tau_{res}}{\sigma_{eq}} M_{ij} + \frac{\xi}{3\overline{\sigma}} \Delta G_{MV}^2 \exp\left(\frac{\sigma_m}{\overline{\sigma}}\right) I_{ij} \right] \end{cases}$$
(37)

(38)

576

 $\dot{\kappa} = \Lambda_p$

577

$$\begin{cases}
\nabla^{ASB} \\
D_{ij} = \frac{3\tau_{res}^{2}}{\sigma_{eq}}\Lambda_{ASB}\eta_{ASB}\Delta G_{ASB}N_{ij} \\
\nabla^{MV} \\
D_{ij} = 3\Lambda_{MV} \left[\frac{\tau_{res}^{2}}{\sigma_{eq}}\eta_{MV}\Delta G_{MV} + 2\xi\Delta G_{MV}\exp\left(\frac{\sigma_{m}}{\overline{\sigma}}\right)\right]N_{ij}
\end{cases}$$
(39)

578 It is to be noted that in the present study void expansion is modelled irreversibly and the 579 void closure which may take place during change of the loading sign is not taken into 580 consideration. The inclusion of ΔG_{MV}^2 in the void expansion term of the yield function 581 translates into ΔG_{MV}^2 and ΔG_{MV} in the corresponding terms of $d_{ij}^{in(MV)}$ and D_{ij}^{VMV} 582 respectively. This ensures the systematic concomitance of the deviatoric and hydrostatic 583 terms of the rate equation relevant to MV.

The components of the deterioration induced spin rates can be deduced from (6) and (37) as:

586

$$\omega_{ij}^{in(ASB)} = 3\Lambda_{P} \frac{\eta_{ASB} \Delta G_{ASB}^{2} \tau_{res}}{\sigma_{eq}} T_{ij}$$

$$\omega_{ij}^{in(MV)} = 3\Lambda_{P} \frac{\eta_{MV} \Delta G_{MV}^{2} \tau_{res}}{\sigma_{eq}} T_{ij}$$
(40)

588 The viscous stress in (35) is assumed of the form:

$$\sigma_{v} = Y \,\dot{\kappa}^{1/n} \tag{41}$$

590 It is reminded that *Y* and *n* are viscous constants corresponding to the regular plasticity 591 and as such do not depend on D.

592 2.2.3.9 Temperature rise

593 The regular temperature rate is calculated from the intrinsic plastic dissipation 594 expressed in (13) assuming adiabatic conditions as:

595
$$\rho c \dot{T} = \tau_{ij} : d_{ji}^p - r \dot{\kappa}$$
(42)

596 As the dissipation progressively concentrates within the band during the ASB process, 597 the regular temperature rate accordingly vanishes and the regular temperature 598 saturates; further cooling during unloading should be accounted for in prospective 599 works.

600 **2.3 DETERIORATION INCIPIENCE CRITERIA**

The mechanisms leading to onset of the ASB and MV and the corresponding criteria adopted are discussed in the current section.

603 2.3.1 Softening mechanisms triggering the ASB formation

604 A criterion for the incipience of the ASB based on the physics of the mechanism is essential. In the literature, several arbitrary ASB incipience criteria have been postulated 605 606 for example based on critical strain, see Zhou et al. [39], strain rate, see Bonnet-607 Lebouvier et al. [14], temperature rise, see Teng et al. [15], and energy, see Dolinski et al. 608 [40]. Although the above mentioned engineering oriented criteria are easy to 609 implement, they strongly depend on the geometry and loading conditions. Hence there is 610 a need for a robust physics based criterion consistent with the constitutive equations. 611 Such a criterion may be obtained from the linear perturbation analysis, see e.g. Anand et 612 al. [41]. Longère et al. developed a criterion as shown in (43) based on simplified 613 analysis of material instability accounting for the competition between hardening and 614 softening mechanisms using the linear perturbation method. A detailed account of this 615 approach can be consulted in the references - Molinari [42], Longère et al. [21], Longère 616 and Dragon [43].

617
$$J\left(\tau_{ij}, r, \dot{\kappa}; \frac{\partial r}{\partial \kappa}, \frac{\partial r}{\partial T}\right) = \sqrt{3}\tau - \left(r - \frac{1}{n}Y\dot{\kappa}^{\frac{1}{n}} + \rho_0 c_0\left(\frac{\partial r}{\partial \kappa} / \left(-\frac{\partial r}{\partial T}\right)\right)\right) \ge 0$$
(43)

618 where $\partial r / \partial \kappa$ represents the strain hardening and $\partial r / \partial T$ the thermal softening effects. 619 The deterioration process is actually assumed to run as soon as J=0. This criterion 620 allows for determining G_{ASB} (= **G** : **N** at the instant of ASB incipience).

Two softening mechanisms triggering the ASB formation are considered in the presentstudy, viz. thermal softening and dynamic recrystallization.

623 2.3.1.1 Thermal softening

At high strain rates, adiabatic conditions can be assumed due to the limited time for heat transfer (see [44]). Thermal softening along with quasi-adiabatic condition plays an important role in provoking the ASB onset. The form of the thermal softening function can be adapted to different materials as shown in (21) and (22). It is therefore essential to accurately calculate the regular temperature rise causing the thermal softening. The plasticity induced regular temperature rise shown in (42) can also be expressed as:

630
$$\rho c \dot{T} = \left(\frac{\sigma_{VM}^2}{\sigma_{eq}} - r\right) \dot{\kappa}$$
(44)

In most studies in the literature, the percentage of plastic work converted to heat i.e. the inelastic heat fraction β is assumed to be constant; for example $\beta = 0.6$ in [45], $\beta = 0.9$ in [46]. However the experiments by Mason et al. [47] show that β is not a constant and varies with the strain, strain rate and temperature (see also [48],[49]) as is potentially the case in the present study. The form of the inelastic heat fraction can be deduced from (44) as:

637
$$\rho c \dot{T} = \beta \sigma_{VM} \dot{\kappa} \quad ; \quad \beta = \frac{\sigma_{VM}}{\sigma_{eq}} - \frac{r}{\sigma_{VM}}$$
(45)

As *r* depends on strain and temperature and $\sigma_{_{V\!M}}$ is a function of strain, strain rate and temperature, β is expected to depend on strain, strain rate and temperature as well, see [50]. During the ASB process, the dissipation progressively concentrates within the bands. Correspondingly, the evolution of the regular temperature outside the bands diminishes and finally saturates.

643 2.3.1.2 Dynamic recrystallization

644 It has been shown that the microstructure also influences the ASB incipience, see eg. Liu 645 et al. [28]. The micro-mechanisms contributing to the regular material softening and 646 influencing the ASB onset, which are taken into consideration in the present study, are 647 the dynamic recovery (DRC) and dynamic recrystallization (DRX). Many studies have 648 shown that the DRX occurs as a consequence of the adiabatic shear banding 649 ([51],[52],[53]). Contrarily, for certain alloys such as those of titanium, DRX is shown to 650 contribute significantly to the softening leading to the very formation of ASB (see 651 [25],[26]). The latter approach is considered in the present work and the competition 652 between the DRX softening and thermal softening provoking the ASB initiation is

studied. The detailed development of the DRX related model can be found in the articleby Longère [30].

For the initial study on DRX, a critical value of the isotropic hardening variable κ_c is imposed to initiate occurrence of DRX. According to Mohamed and Bacroix [54], the stored energy at DRX onset should depend on temperature. But in the present study, for simplification, κ_c is maintained constant and temperature independent. The DRC and DRX induce a negative hardening effect (softening) and it is modelled in the hardening term $h'(\kappa)$ as shown in (46).

661
$$h'(\kappa) = \tau_s \left(Y(\kappa) \right) \left[1 - \exp\left(-\frac{Y(\kappa)}{2} \kappa \right) \right]$$
(46)

662 τ_s is the DRC and DRX dependent saturation value of hardening stress. $Y(\kappa)$ is a non-663 dimensional quantity phenomenologically composed of DRC and DRX components 664 expressed below.

665
$$Y(\kappa) = Y_{DRC} + Y_{DRX}(\kappa); \quad \tau_s(Y(\kappa)) = \frac{\eta}{Y(\kappa)}$$
(47)

666 where

667
$$\begin{cases} Y_{DRC} = Y_0 \\ Y_{DRX} = Y_{max} \left[1 - \exp\left(-\frac{\left\langle \kappa - \kappa_c \right\rangle}{\Delta \kappa_r}\right) \right] \end{cases}$$
(48)

668 η and $\Delta \kappa_r$ are kinetics related constants. $Y_{DRC} = Y_0$ is considered a constant. Y_{max} 669 represents the saturation value of the quantity Y_{DRX} .

670 2.3.2 Mechanisms triggering the MV formation

The micro-voiding triggered during the loading and after unloading are distinguishedhere.

673 • During loading

Micro-voids can nucleate during the ductile damage process in several ways. The voids primarily nucleate around inclusions [55] and also at the grain boundary triple points [56] in the material. The void nucleation may be triggered by the particle-matrix interface decohesion, the particle rupture or micro-cracking of the matrix around the particle [57].

679 • After unloading

As mentioned in section 2.1.1.2, the phase transformation due to quenching of the ASB
after unloading provokes the formation of micro-crack at the ASB/matrix interface. The
question arises whether the micro-cracks observed by Peirs et al. [1] within the ASB are
formed during or after the loading.

The case treated in the current work is effect of MV during the characteristic loading time. In absence of further analytical tools or experimental data, the micro-voiding is tentatively assumed to initiate as soon as the ΔG_{ASB} reaches a transition-tovoiding/critical level ΔG_{ASB}^{crit} such that $G_{MV} = \text{Tr}(\mathbf{GN})_{MV} = G_{ASB} + \Delta G_{ASB}^{crit}$. The ΔG_{ASB}^{crit} is calculated as $\Delta G_{ASB}^{crit} = (\Omega - 1) * G_{ASB}$ where Ω is tentatively an arbitrary constant greater than unity. After the MV initiation, ΔG_{ASB} is maintained constant at the value of ΔG_{ASB}^{crit} and ΔG_{MV} evolves taking the predominance as the degradation driving force.

691 3 NUMERICAL IMPLEMENTATION AND PERFORMANCE 692 EVALUATION

693 The model in itself does not represent the ASB and MV as entities in the finite elements 694 but it phenomenologically reproduces their consequences in the elements. For a model 695 to be considered predictive, it has to satisfy a complete Verification and Validation (V&V) procedure, (see [20]), which consists in numerically evaluating the performances 696 697 of the model on initial boundary value problems (IBVP) with increasing complexity against corresponding experimental results. In the literature, the models describing ASB 698 are widely calibrated and evaluated using a single IBVP. Indeed, the high strain rate 699 700 loading of a hat shaped structure (HSS) is often used to this end, but this should not be 701 considered as a sole evaluating configuration as the ASB orientation and path are 702 entirely controlled by the specimen geometry and the predictability of the model cannot 703 be sufficiently assessed.

In the (V&V) procedure, the model is first numerically implemented at the scale of a representative volume element (RVE) in order to determine the viscoplasticity and

706 viscous deterioration related constants for a given material from simple experimental 707 results such as those of standard tension/compression tests at various temperatures 708 and strain rates along with high strain rate torsion or/and shear tests. This is the step of 709 material constants calibration. The model performance is then evaluated and the constants are further adjusted if needed by considering an initial-boundary value 710 711 problem (IBVP) for example using a structure, e.g. HSS [4] or Kalthoff and Winkler (KW) 712 impact specimen ([58],[59]), as the ASB path in these structures is known a priori. The 713 set of material constants is expected to satisfy the experimental results obtained from 714 both the simple tests and the tests on the structures. This is the step of **verification**. The 715 final challenging **validation** step is to test the model on a more complex structure where 716 the shear band path is a priori unknown, for example, ballistic impact of a thick plate [4], 717 high speed machining, etc.

718 In the present work, due to the lack of quantitative experimental results concerning the 719 MV, instead of the V&V, the feasibility and robustness of the enriched model is 720 demonstrated on the RVE and structural scale. The implementation of the model on the 721 complex IBVP namely simulation of high speed machining is a work in progress.

722 3.1.1 Numerical issues

Dealing numerically with this local softening phenomenon, resulting from a competition between material hardening and softening mechanisms and which has severe irreversible consequences at the structural level, still remains a challenging task. Indeed, the aim is to control the evolution of this material instability all along its progress and accordingly overcome the numerical instability the finite element computation code is subject to in the softening regime and subsequent meshing dependence of the numerical results.

Explicit time integration schemes are considered for both the initial-boundary value
problem and rate equations of the constitutive model. In other words, the finite element
computation code, namely LS-DYNA, is explicit and the rate equations are integrated
within a user material subroutine according to an explicit time integration scheme. The
numerical analyses are carried out using brick finite elements (continuum, 3-D, 8-node,
reduced integration).

The nonlinear constitutive model implemented as 'user material' subroutine is governedby a system of differential equations which can be written as (see also [60])

738
$$\dot{F} = A(F,t)F + f(F,t) \quad ; \quad F = F(v,\rho,\tau,r,\tilde{\mathbf{G}},\tilde{\mathbf{D}},T)$$
(49)

739 where A(F,t) represents a linear differential operator, and f(F,t) a nonlinear 740 function. The forward finite difference method has been used to integrate the above 741 equations. In the framework of the present study, numerical stability and convergence 742 are furthermore controlled by an adaptive time sub-increment procedure based on the 743 maximum strain increment $\Delta \overline{e}$ principle (see [61]):

744
$$\overline{\Delta t} = \frac{\Delta \overline{e}}{\dot{\overline{e}}} ; \dot{\overline{e}} = \sqrt{\frac{2}{3} d_{ij} d_{ji}}$$
(50)

where $\overline{\Delta t}$ represents the adaptive time sub-increment, $\dot{\overline{e}}$ a scalar measure of the 745 746 current strain rate, and $\Delta \overline{e}$ the numerical admissible maximum strain increment. According to (XX), the value of $\overline{\Delta t}$ is dependent on the current strain rate in the element. 747 We are designating Δt_{CFL} the time increment imposed by the explicit computation code 748 LS-DYNA calculated with respect to Courant-Friedrichs-Lewy [62] condition for wave 749 propagation. As long as $\Delta t_{CFL} < \overline{\Delta t}$, the value of $\overline{\Delta t}$ is forced to be equal to the value of 750 $\Delta t_{\rm \it CFL}$, which ensures the numerical stability and convergence from the viewpoint of the 751 numerical integration of the constitutive equations. At high strain rate, the value of $\overline{\Delta t}$ 752 could become lower than the value of Δt_{CFL} . In this case, and for the element concerned, 753 the sampling procedure is activated, using an optimised integration time increment such 754 as $\overline{\Delta t}_{opt} = \frac{\Delta t_{CFL}}{N}$, $N = Int\left(\frac{\Delta t_{CFL}}{\overline{\Delta t}}\right) + 1$. The optimised integration time step is determined 755 756 as follows :

757
$$\overline{\Delta t}_{opt} = \frac{\Delta t_{CFL}}{N} \text{ with } \begin{cases} N = 1 & \text{if } \Delta t_{CFL} \le \overline{\Delta t} \\ N = Int \left(\frac{\Delta t_{CFL}}{\overline{\Delta t}}\right) + 1 & \text{if } \Delta t_{CFL} > \overline{\Delta t} \end{cases}$$
(51)

This procedure involves a sub loop for the concerned elements only. Considering the
great number of elements, this last point is crucial with regards to the calculation and
(storage and dynamic) memory costs."

The flow chart describing the different steps of the algorithm is depicted in Fig. 9.



- 762
- 763

Fig. 9 Flow-chart of the algorithm

764 3.1.1.1 Regularization and mesh dependence

The viscosity (rate dependency of both plasticity and degradation mechanisms) contributes to regularize the boundary vale problem in the softening regime, see [63], [64]. Yet, as the ASB induces a very strong local softening, additional measures need to be applied to overcome the numerical instability. For this purpose, an adaptive time subincrement procedure based on maximum strain increment principle (see [61],[29]) is imposed which consists in partitioning the global time increment to obtain a local time increment used to integrate the constitutive equations on the concerned elements.

772 Due to the usage of large scale postulate in the model, an a priori knowledge of the shear 773 band path and hence mesh refining in the selected regions is not required. A study on 774 the influence of the mesh size of the initial model describing the effect of ASB was 775 carried out by Longère et al. [29] and [4]. The large scale postulate requires the ASB to be embedded within the finite element which in turn implies that it is not feasible to use mesh of any given size. It was shown that a mesh size of approximately five times the shear band (\sim 500µm for high strength steel) width satisfies the scale postulate. A very coarse meshing would give rise to a dispersed area of deteriorated finite elements.

780 *3.1.1.2 Band orientation*

According to experimental observations, the ASB is oriented in the plane of the maximum shear stress. This requires the information of the principal stress values. With the knowledge of the plane of maximum shear stress, the resolved shear stress τ_{res} and normal tension stress σ_N are calculated.

785 3.1.1.3 Stress triaxiality

The ASBs are formed and propagate under conditions of negative or zero stresstriaxiality. Accordingly, in the user material subroutine, an external condition is imposed

such that the incipience of ASB and the evolution of \mathbf{D} take place only under positive or nil pressure.

790 On the other hand, different arguments have been proposed in the literature regarding 791 the stress triaxiality conditions for the formation and growth of micro-voids. Bao and 792 Wierzbicki [65] stated that the micro-voids occur only under positive stress triaxiality 793 and they transform into micro-shear decohesion under an asymptote of -1/3 negative 794 stress triaxiality. However, Longère et al. [27] demonstrated that the micro-voids could 795 initiate and grow around inclusions in the material even under shear pressure loading. 796 The latter view point is adopted herein and hence in the user material subroutine, the 797 MV mechanism is allowed to operate both under negative and positive pressure 798 conditions. The MV expansion is also minimally active in the negative stress triaxiality 799 condition, thanks to its exponential dependence on the mean stress whose form is 800 adopted from Rousselier [33] which itself is derived from Rice and Tracey [38].

801 3.1.1.4 Crack formation

A material failure criterion is required in order to numerically process the element deletion. A theoretical upper bound for \mathcal{D} from (2) exists considering melting point of the material as the maximum temperature limit which is explained in [21]. The crude theoretical approximation for critical deterioration intensity $\mathcal{D}_c = \mu/b$ is shown in (19).

- Numerically implementing the D_c as a threshold for element failure is not feasible as the
- 807 elements would undergo excessive distortion (even though LS-DYNA is able to deal with
- 808 large distortion) at such high values of \mathcal{D} . Therefore currently an upper limit for $Tr\mathbf{D}$ is
- 809 imposed in the user subroutine as a criterion for element deletion. It is to be noted that
- 810 the numerical simulation of the crack propagation still remains a challenge and it could
- be dealt with X-FEM in the future, see for example [66], [67], [68], [69].

812 3.2 NUMERICAL IMPLEMENTATION ON RVE SCALE

813 The enlarged ASB+MV model is herein numerically implemented on a 3 dimensional 814 RVE i.e. a single brick finite element of *H*-length. The FE is clamped on the bottom and

815 tangentially loaded on the top with a velocity *V* producing simple shearing. The shear

816 strain Γ used in the following is defined as $\Gamma = \int \dot{\Gamma} dt$ where $\dot{\Gamma} = V / H$. Two cases are

817 studying in the following corresponding to two typical materials susceptible to ASB: high 818 strength steel for which the ASB onset is controlled by thermal softening and high 819 strength titanium alloy for which there is a competition between/combination of

820 thermal softening and DRX for the ASB initiation.

821 3.2.1.1 High strength steel: Thermal softening-controlled ASB onset

The material under consideration is high strength 30 Ni-Cr-Mo 6-6 type steel. The constants pertaining to plasticity and hardening are mostly obtained from [4]. The constants related to the ASB and MV induced softening are assigned arbitrary values in the current performance study.

| 827 | Elastic - vi | scoplastic c | onsta | ants: | | | | | | |
|-----|----------------------------|-----------------------------|----------------|------------------------------------|---------------------|------------------------|--------------------|---------------------------------|--------------------|---|
| | $\rho_0 \ (\text{kg/m}^2)$ | ³) c_0 (J/kg. | K) | E (MPa) | ν | $R_{\infty}(M)$ | IPa) | R _{int} (MPa) | $Y (MPa. s^{1/n})$ | n |
| | 7800 | 420 | | 200e+3 | 0.33 | 400 | 0 | 920 | 60 | 6 |
| 828 | Thermal properties: | | | | | | | | | |
| | | | k | v (°C ⁻¹) | T_0 (°C | $\overline{\alpha}$ (/ | /K) | $\dot{\mathcal{E}}_{crit}$ (/s) | | |
| | | - | 10 | 1.1e-3 | 20 | 1e- | -6 | 100 | | |
| 829 | AS | B related co | nstar | nts: | | | | | | |
| | | Z (MPa. s ^{1/n}) |) m | $\eta_{\scriptscriptstyle ASB}$ (M | [Pa ⁻²) | χ_1 | χ_2 | a (MPa) | b (MPa) | |
| | | 15 | 2 | 0.0 | 1 | 0.04 | 0.04 | 0 | 15e+3 | |
| 830 | | MV | relat | ed consta | nts: | | | | | |
| | | | $W(\mathbf{N}$ | (IPa. $s^{1/n}$) | q η | _{MV} (MP | °a ⁻²) | ξ Ω | | |
| | | - | | 20 | 2 | 0.08 | | 1 1.5 | | |

| 826 | Table 2 Material properties for 30 Ni-Cr-Mo 6-6 type steel |
|-----|--|
|-----|--|

831 The shear stress – shear strain plot for three different cases of material model are shown 832 in Fig. 10. The response of polycrystalline plasticity material without any localization is shown by the solid blue line. The thermal softening induced slight and smooth drop in 833 834 strength is seen in this case. The model considering ASB induced deterioration is shown 835 by the red dotted line in which we see a strong drop in strength after ASB onset. The 836 purple dashed line represents the enriched ASB+MV model in which a relatively more 837 abrupt drop in strength is observed due to the additional MV contribution. The drop in 838 stress is attenuated by the viscosity of both ASB and MV. In other words, increasing the 839 velocity, results in a less brutal drop in stress with a smoother slope. The inertial effects 840 which are known to play an important role during void growth, see e.g. [70], are not 841 explicitly accounted for in the present model, but their regularizing consequences are at 842 least partly reproduced thanks to the viscous feature of the MV process. The constants 843 pertaining to the MV in Table 2 are chosen in such a way so as to magnify its effect on 844 the material and kinematics for the sole purpose of visualization.



Fig. 10 Shear stress vs Shear strain plots for models with i) polycrystalline plasticity only, ii) plasticity
 +ASB and iii) plasticity+ ASB+MV

848 The evolution of the deterioration driving force containing quantities $G = \tilde{G}$:N and ΔG 849 are shown in Fig. 11. Comparing *G* versus shear strain for ASB and ASB+MV cases, in Fig. 850 11a, the additional MV induced contribution to *G* after its onset in the ASB+MV model 851 can be clearly seen. For the ASB+MV model, the progression of ΔG_{ASB} and ΔG_{MV} is plotted in Fig. 11b. After attaining the critical value ΔG_{ASB}^{crit} , ΔG_{ASB} remains constant 852 853 while ΔG_{MV} initiates and grows. The fact that ΔG_{ASB} is non zero when MV operates 854 allows the ASB-related process to operate until vanishing. In other words, MV becomes 855 progressively and not suddenly predominant, as shown later.

856



Fig. 11 Deterioration driving force vs. Shear strain (a) G:N for models with ASB only and ASB+MV; (b) ΔG
 for the ASB+MV model showing the two components

For the ASB+MV model, the total inelastic strain rate d_{12}^{in} and its various components vs the shear strain are shown in Fig. 12. Initially, the d_{12}^{in} is composed of the "regular" polycrystalline plastic strain rate. At the onset of shear localization regular contribution diminishes and the "singular" plastic strain rate becomes progressively predominant. The singular part is composed initially of the ASB induced strain rate $d_{ij}^{in(ASB)}$ and later by the MV induced strain rate $d_{ij}^{in(MV)}$.



866 867

857

Fig. 12 Inelastic shear strain rate with its components for the ASB+MV model

868 The evolution of the total deterioration rate $Tr(\mathbf{D}^{\nabla^{ASB+MV}})$ with its ASB and MV 869 components are presented in Fig. 13a. Finally, Fig. 13b shows the trace of the 870 deterioration tensor for ASB and ASB+MV models. The significant addition to the Tr**D** 871 due to MV is clearly seen.



Fig. 13 (a) ASB+MV model: Deterioration rate with its components; (b) TrD for ASB only and ASB+MV models
 B73



The DRX mechanism is predominantly found to occur in Ti-6Al-4V as a potential cause of softening leading to the formation of ASBs [25]. In this section the enriched ASB+MV constitutive model containing DRX aspects is implemented on the RVE scale i.e. a single brick finite element for the Ti6Al4V alloy. The material properties concerning viscoplasticity and the thermal properties are obtained from experimental results as observed in [30]. The ASB, MV and DRX constants are assigned arbitrary values for the current parametric study.

882 **Table 3** Material properties for Ti-6Al-4V

883 Elastic - viscoplastic constants:

| P_0 (kg/m) C_0 (J/kg/k) E (MFa) V K_{∞} (MFa) K_{int} (MFa) | Y (MPa. s ^{1/n}) | п |
|--|----------------------------|----|
| 4500 460 113e+3 0.34 972 1080 | 400 | 44 |
| 884 Thermal properties: | | |
| $T_0(^{\circ}\mathrm{C})$ $\overline{lpha}(/\mathrm{K})$ $T_{ref}(\mathrm{K})$ t $\dot{\mathcal{E}}_{crit}(/\mathrm{s})$ | | |
| 20 1e-6 923 0.6 100 | | |
| ASB related constants: | | |
| Z (MPa. s ^{1/n}) $m \eta_{ASB}$ (MPa ⁻²) $\chi_1 \chi_2 a$ (MPa) | <i>b</i> (MPa) | |
| 100 2 0.01 0.04 0.04 0 | 15e+3 | |
| 886 MV_related constants: | | |
| W (MPa. s ^{1/n}) $q \eta_{MV}$ (MPa ⁻²) $\xi \Omega$ | | |
| 75 2 0.05 1 2 | | |
| 887 DRX related constants: | | |
| $Y_0 Y_{\max} \kappa_c \Delta \kappa_r \eta (\text{MPa})$ | | |
| 14 14 0.2 0.8 1.36e+4 | | |

In line of the work by [30] dealing with ASB only, the competitive influence of the two softening mechanisms provoking the formation of the ASB, namely thermal softening and DRX induced softening, and their effects on MV are studied here. Four different cases are numerically studied here :

- 892 (1) no thermal softening and no DRX (No TS & No DRX)
- 893 (2) no thermal softening and with DRX (No TS & With DRX)
- 894 (3) with thermal softening and no DRX (With TS & No DRX)
- 895 (4) with thermal softening and with DRX (With TS & With DRX)

896 The DRX related constants are chosen such that the ASB incipience and consequently the 897 start of the drop in strength take place almost at the same time for cases (2) and (3). Fig. 898 14 shows the plot of shear stress vs shear strain for the four different cases. For the first 899 case, when no softening mechanism comes into play, no material degradation takes 900 place as expected. The ASB incipience instant is marked by a red spot and MV incipience 901 by a green one on the curves. It is seen that as calibrated, the ASB incipience takes place 902 more or less simultaneously for cases (2) and (3) i.e. cases incorporating thermal 903 softening only or DRX softening only. When both the softening mechanisms act in case 904 (4), it is seen that the ASB onset takes place much earlier. The MV onset on the other 905 hand is not directly influenced by the softening mechanisms but it depends on the value 906 of G_{ASB} according to the current model.



907



909 3.3 APPLICATION TO INITIAL BOUNDARY VALUE PROBLEMS

910 Following the V&V principle, the feasibility of the enriched ASB+MV model on an IBVP is 911 demonstrated by simulating the dynamic shearing of a hat shaped structure (HSS). A 912 Couque type HSS [71] (see Fig. 15a) is used to this end. When the HSS is impacted, the 913 inclined gauge section permits constant positive pressure and shear loading creating 914 negative stress triaxiality conditions and thereby making it conducive for ASBs to form. 915 Thus the ASB trajectory (i.e. gauge section) is known a priori and the HSS is suitable for 916 verification of the model. Simulations are carried out for impact of HSS in a direct 917 Hopkinson bar setup made up of tungsten, with a striker bar velocity of 30 m/s; see Fig. 918 15.





920 3.3.1 Case of High Strength Steel

As it is the case of steel, only thermal softening is taken into account as the softening mechanism leading to the formation of ASB. The ASB and MV related material constants used here for 30 Ni-Cr-Mo 6-6 steel are shown in Table 2. As in the elementary responses of the RVE examined in section 3.2, two configurations are studied in the following: (i) configuration describing ASB effect only, i.e. with MV onset being deactivated, and (ii) configuration reproducing both ASB and MV effects where ASBrelated constants are the same as those used in (i).

Firstly, the resolved shear stress τ_{res} is examined as function of time for the elements in the gauge section, as shown in **Fig. 16**, of the HSS. The ASB model shows a relatively mild drop in strength in Fig. 17a after the ASB onset whereas the loss of strength is accelerated by the presence of MV in Fig. 17 for the ASB+MV model.



Fig. 17 Numerical simulation of the dynamic loading of hat shaped structure. Model: ASB only. a) Resolved
 shear stress history. b) Deterioration variable history. See Fig. 16. for the location of the elements.

- 936 The evolution of the deterioration variable $Tr\mathbf{D}$ for ASB and ASB+MV is plotted in Fig.
- 937 18,18b. As expected, the deterioration intensity is significantly higher for the ASB+MV
- 938 case when compared with the ASB only model.



Fig. 18 Numerical simulation of the dynamic loading of hat shaped structure. Model: ASB +MV. a)
Resolved shear stress history. b) Deterioration variable history. See Fig. 16. for the location of the elements.

The numerical deterioration maps shown in the following give an indication of the presence of ASB/MV in the finite elements. In Fig. 19, for the model considering ASB only, the elements in red contain ASB. Likewise for the ASB+MV model in Fig. 20, the elements with ASB are highlighted in red (Fig. 20a) and the ones containing MV in blue (Fig. 20b).



947

Fig. 19 Model with ASB only: Deterioration indicator at 39µs. Elements in red are subjected to ASB.



Fig. 20 Model with ASB+MV: Deterioration indicator at 39μs. a) Elements in red are subjected to ASB. b)
 Elements in blue are subjected to MV.

951 These numerical results bring two comments. Firstly, at the same time, considering ASB 952 only leads to a partial propagation of ASB in the gauge section (Fig. 19), whereas 953 considering both ASB+MV leads to a complete propagation of ASB (Fig. 20). MV in ASB 954 wake thus contributes in propagating the ASB farther. Secondly, according to Fig. 20 and 955 assuming that the loading ends at the time considered, although ASB has propagated 956 throughout the whole structure, MV zones cover very limited areas, viz. near the 957 specimen corners. . The material in the ligament between the MV zones, which has been 958 subject to ASB, may recover its initial properties after unloading due to phase 959 transformation. In other words, the remaining effect of ASB+MV may reduce to MV alone 960 with only local parts of the structure affected. In another scenario, the quenching of the 961 material of ASB after unloading and cooling may cause micro-cracking, leading to a 962 complete fracture of the structure.

963 **3.3.2 Case of Ti6Al4V**

964 As mentioned in Section 2.3.1.2, the works of Rittel and co-workers [25] suggest that, for 965 materials such as high strength Ti alloys, the phenomenon of dynamic recrystallization 966 (DRX) potentially needs to be taken into account in ASB initiation. Unlike the common 967 assumption that DRX is a consequence of ASB, they argue that the DRX not only precedes 968 the ASB but is also a dominant microstrutural factor in the very generation of the band. 969 Osovski et al. [45] concluded that the respective influence of thermal and DRX induced 970 softening depends on the chronology of the process and the material considered: in case 971 of Ti6Al4V, DRX develops earlier and overrides the thermal softening effects; on the 972 other extreme case of pure titanium which does not undergo DRX, the thermal softening 973 plays a dominant role in the ASB initiation. In the line of their work, the competition 974 occurring between thermal and DRX induced softening is analyzed here on a structural 975 scale. The materials constants of Ti6Al4V are shown in Table 3.

- 976 In order to study the potential effect of DRX on ASB formation and evolution, two cases
- 977 are examined in the simulation of HSS:
- 978 (1) no thermal softening and with DRX (No TS & With DRX)
- 979 (2) with thermal softening and with DRX (With TS & With DRX)
- 980 These configurations have to be considered together with those studied in Section981 3.2.1.2.

982 The resolved shear stresses for both cases for the selected elements in the gauge section 983 (as shown in Fig. 16) of the HSS are plotted in Fig. 21a,b. In the graphs, the red marks 984 indicate the ASB onset and the green ones MV onset. While examining the two cases for 985 the instant of ASB onset, it is clearly seen that the case with combined DRX and thermal 986 softening (Fig. 21b) shows relatively early onset of ASB when compared to the case of 987 DRX induced softening only (Fig. 21a). Consequently the MV onset also takes place 988 earlier for the former case than the latter. The results seen here is similar to the ones 989 observed in the corresponding cases for the single FE in Chapter 2, Section 2.5.2.2.

The deterioration maps showing the elements with ASB and MV activated respectively at a given instant (viz. 45µs) for the above two cases are shown in Fig. 22. In the case considering DRX induced softening solely (Fig. 22a), fewer elements show ASB and MV at the given instant. The combined influence of thermal and DRX induced softening seems to have accelerated the ASB and MV onset which is seen in the deterioration map (Fig. 22b) in which relatively more elements are seen with the presence of ASB and MV.

As a consequence, neglecting the thermal softening and considering only DRX induced
softening for materials such as Ti6Al4V as proposed by Osovski et al. [45], would lead to
delay of ASB initiation and underestimation of the ASB propagation. However more

999 experimental evidence is needed to characterize each material in terms of the respective1000 influence of thermal and DRX induced softening on the shear localization onset.



Fig. 21 Model ASB+MV: Deterioration variable history of elements in the gauge section, see Fig. 16. a)
 Case of no thermal softening and with DRX b) Case considering thermal softening and DRX.

1003 **3.3.3 Experimental vs. numerical results confrontation**

In order to assess the prediction ability of the model to describe ASB and further microvoiding, numerical results are compared with experimental ones. Material constants are
reported in Table 4. Two configurations extracted from [4] are considered in the present
work:



1012 In the moderate impact configuration, see Fig. 23 left, ASBs are shown to form from the 1013 specimen corners and propagate partially. A small crack has formed in the ASBs wake. In Fig. 23 right related to the numerical simulation, the same trend is observed where the 1014 1015 damaged area length is slightly smaller than the ASB length. In the severe impact configuration, see Fig. 24 left, ASBs initiated from the corners join together to form a 1016 1017 single band as do the cracks, leading to the complete fracture of the specimen. The same 1018 trend is observed once again in the numerical simulations. The comparison of the 1019 experimental macrograph, on the left, with the ASB and MV indicator maps, on the right, 1020 and of the history of the experimental and numerical axial stress on the left allows for 1021 concluding to a fair agreement.





1025 3.3.4 Discussion/assessment

1026 The realistic description of initiation and propagation of ASB and MV and their 1027 consequences on the structural material in a wide range of situations implies modelling 1028 as close as possible to the complex physics of the mechanisms while being tractable and 1029 applicable to initial boundary value problems. The enriched ASB+MV three-dimensional 1030 constitutive model is herein demonstrated to be feasible on a structural scale and shows 1031 the desired qualitative performance on the IBVP.



Axial stress transmitted into the output bar

Fig. 23 Configuration with L_{striker}=90mm ; V_{striker}=23.7m/s. Incomplete ASB and MV propagation. left: Post mortem macrograph and Axial experimental and numerical stress transmitted into the output bar ; right:
 Numerical deterioration map (100 μs).

• ASB only vs. ASB+MV

- 1041 While comparing the two models exhibiting ASB only and ASB+MV when implemented 1042 on a structural scale, the following conclusion can be drawn. The model with ASB and 1043 MV activated exhibits increased deterioration intensity and therefore accelerates the 1044 drop in strength of the material which is the expected behaviour. Also, while comparing 1045 with the ASB only model, the presence of MV advances the ASB propagation.
- 1046 Not all elements containing ASB show the presence of MV at a given instant. This would
- 1047 imply that, upon loading at that given instant, if the material within the ASB recovers its
- 1048 initial properties due to phase transformation, the only deteriorated region would be the
- 1049 elements containing MV. It is thus essential to distinguish the two mechanisms of ASB
- 1050 and MV.





ASB indicator map



MV indicator map

Axial stress transmitted into the output bar



- 1054
- 1055 DRX vs. DRX+TS

1056 In case of materials susceptible to DRX such as high strength Ti alloys, in addition to 1057 thermal softening, the DRX induced softening plays a role on the ASB onset. The 1058 influence of the two softening mechanisms has been studied here concerning two cases 1059 namely DRX only and DRX+TS. It is seen that the combined DRX+TS leads to a much 1060 earlier onset of ASB and consequently MV when compared to the case with DRX induced 1061 softening only. It is therefore important to consider both the softening mechanisms in 1062 order to be conservative in the engineering approach.

1063 4 **CONCLUSION**

A physics motivated phenomenological model describing ASB and MV effects developed 1064 1065 in a large scale postulate has been applied herein in accordance with the physics of the shear localization and subsequent ductile damage process. The two main effects of 1066 1067 ASB+MV induced deterioration reproduced by the unified model are: material 1068 consequence, viz. anisotropic deterioration of the material elastic and plastic properties; 1069 and kinematic consequence, viz. progressive deviation of the plastic flow in the band 1070 plane and then according to the micro-void orientation. The present enlarged ASB+MV 1071 model is numerically implemented as user material in the engineering finite element 1072 computation code LS-DYNA. The model has been successfully demonstrated to be 1073 numerically feasible at the representative volume element scale and also on a structure 1074 namely the hat shaped structure (HSS). The ASB+MV model distinguishes the ASB and 1075 MV induced effects in the late pre-failure stage and the supplementary MV contribution 1076 to the deterioration could be observed.

The qualitative analysis of the ASB+MV model is done by comparing with ASB only 1077 1078 model in which the MV is deactivated while maintaining the ASB related constants. On 1079 the scale of the RVE, the ASB+MV model demonstrates the desired behaviour by 1080 showing supplementary MV induced material deterioration and kinematics. On the HSS, 1081 it is observed that the presence of MV accelerates the propagation of ASB which has not 1082 been shown in literature and thus constitutes a novel result. Also, at a given instant, not 1083 all elements containing the ASB reach the criteria for MV onset; only the corner elements 1084 show the presence of MV. One could infer the following possible scenarios from the 1085 given state of elements on unloading: the material within the ASB might recover its 1086 initial properties after being quenched by the surrounding material and thus phase 1087 transformed leaving only the effect of MV in the respective elements in the corners; or 1088 the cooling on unloading might cause micro-cracking within the ASB leading to complete 1089 fracture. The respective influence of thermal and dynamic recrystallization (DRX) 1090 induced softening is also studied on the RVE and structural scale. In both the cases it is 1091 shown that the combined contribution of thermal and DRX softening brings about an 1092 earlier ASB onset as expected. Considering only one of the softening mechanisms would delay the ASB onset and underestimate the ASB propagation, which is in contradiction
with some assumptions in literature considering that DRX is the unique mechanism
controlling the ASB onset particularly in Ti-6Al-4V titanium alloy.

1096 The challenge still remains in terms of identifying the instant of MV incipience from 1097 experiments and hence to distinguish ASB and MV related material constants. Also, in 1098 order to account for the different orientation of the MV with respect to ASB, 1099 experimental observations are required.

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