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Subgrain lath martensite mechanics: A numerical–experimental analysis

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Abstract

Lath martensite reveals a specific hierarchical subgrain structure, with laths, blocks and packets of particular crystallography. The presence of interlath retained austenite layers has been reported in the literature. This paper investigates the potential influence of the interlath retained austenite on the mechanical behaviour of lath martensite subgrains. To this purpose, a martensite grain substructure is modelled using a crystal plasticity framework, with a BCC lath–FCC austenite bicrystal at the fine scale. The main novel contribution of this work is the validation of the hypothesis on the role of the interlath retained austenite in lath martensite using the experimental results reported in the literature. The main features of the experimentally observed deformation behaviour (stress–strain curve, slip activity and roughness pattern) are qualitatively well reproduced by the model. It is shown that the presence of austenite interlath films has the potential to remarkably enhance the local deformation of martensite. In spite of its minor volume fraction, it plays a major role in the orientation dependent mechanical behaviour of the aggregate. It is also shown that if the presence of interlath austenite is neglected, the observed experimental flow curves are not captured.

1. Introduction

The design of advanced high strength steels (AHSS), which are characterised by both good strength and formability, dates back to the early 1970s (see e.g. Rashid, 1981 for the case of Dual Phase steels). In the past decade, their development increased even further by a growing demand for lightweight vehicles and new safety standards.

Lath martensite is one of the main constituent phases in a number of AHSS, such as martensitic steels (Mine et al., 2013), Dual Phase (DP) steels (Cai et al., 1985; Steinbrunner et al., 1988; Calcagnotto et al., 2010) and other multi-phase steels (e.g. low alloyed TRIP steels (Jacques et al., 2007)). Beyond multiple applications in the automotive area, lath martensite is also used e.g. in MEMS (Mine et al., 2013). However, its mechanical behaviour still raises questions (Michiuchi et al., 2009).

Most modelling work on multiphase steels presented in the literature considers lath martensite as a hard, sometimes elastic isotropic phase (Sun et al., 2009; Uthaisangsuk et al., 2011). However, clear evidence exists of the strongly orientation dependent mechanical behaviour of martensite (Mine et al., 2013; Ghassemi-Armaki et al., 2013). Moreover, a number of papers (Cai et al., 1985; Steinbrunner et al., 1988; Calcagnotto et al., 2010; Ghadbeigi et al., 2010; Mine et al., 2013) report evidence of ductile deformation and fracture behaviour of lath martensite under uniaxial tension. This observation seems in

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contradiction with the commonly accepted low ductility of the BCC/BCT martensitic phase. Therefore, the following question arises: what governs the lath martensite orientation dependent, apparently ductile behaviour?

A deeper analysis of the lath martensite deformation mechanisms contributes to the further understanding of its damage and fracture behaviour, and may enhance the exploitation of its potential in technological applications.

To address this question, we depart from the current knowledge on the crystallography and morphology of lath martensite. Recent EBSD and TEM studies (Morito et al., 2003, 2006, 2011) have reported extensive evidence of the hierarchal crystalline substructure of low carbon lath martensite. During quenching from austenite, body centered cubic (BCC) laths and group together according to a specific orientation relationship (approximately Kurdjumov–Sachs) with the parent austenite face centered cubic (FCC) lattice. The lath morphology and the crystallographic relation between multiple martensite subgrains can influence the local and overall anisotropic mechanical behaviour (Hatem and Zikry, 2009; Mine et al., 2013; Maresca et al., 2014). Also, since the martensitic transformation is never complete (Law and Edmonds, 1980; Samuel, 1985; Morito et al., 2011), any interlath austenite films may be retained at lath boundaries. Their presence has been detected by TEM in lath martensite in a number of low carbon steels, e.g. martensitic (Law and Edmonds, 1980; Samuel, 1985; Morito et al., 2011), also tempered (Lee and Su, 1999), stainless steels (Nakagawa and Miyazaki, 1999), DP steels (Kim and Thomas, 1981; Rao and Sachdev, 1982; Jha and Mishra, 1999; Baltazar Hernandez et al., 2011; Kim et al., 2012), low alloyed TRIP steels (Nayak et al., 2012; Song et al., 2012).

We have recently shown (Maresca et al., 2014) that, provided there are enough carriers for plasticity, even a small fraction (5%) of FCC interlath retained austenite can influence the orientation dependent mechanical behaviour of lath martensite at the level of laths with approximately the same orientation. In particular, when shear is applied parallel to the BCC–FCC interface, localised plastic slip occurs in interlath austenite, leading to a remarkable increase of the overall deformation for a given stress level. This result is not just a mere consequence of the fact that the critical resolved shear stress (CRSS) of the FCC phase is lower than that of the BCC phase, but it is intrinsically related to the γ austenite α′ martensite orientation relationship, which is characterised by a habit plane of the approximately ⟨111⟩, family. Hence, there are always 3 slip systems in the FCC phase which are parallel to the BCC–FCC interface, i.e. they are most favourably oriented for carrying plastic slip along the interface.

So far, there was no direct experimental evidence of the role played by interlath retained austenite on the orientation dependent mechanical behaviour of lath martensite. The recent work of Mine et al. (2013) is here used to assess the possible role played by the interlath retained austenite in the mechanical behaviour of lath martensite. In Mine et al. (2013), micrometer-sized tensile specimens were fabricated from a fully lath martensitic low carbon, low alloyed steel. The crystallography of the specimens was identified by means of EBSD before performing mechanical tests. The specimens were strained up to fracture under quasi-static conditions, at room temperature. Stress–strain curves were calculated and surface undulations were measured by scanning white-light interferometry for some strain levels. It is shown that, in all cases, lath martensite does not lose ductility. Moreover, it is observed that slip occurs along lath habit planes at critical resolved shear stresses (310–360 MPa) that are lower than those related to the ⟨112⟩, slip family in BCC laths (500–560 MPa). Slip systems parallel to lath habit planes, also named “in-lath–plane” slip systems are identified in Mine et al. (2013) with slip family ⟨110⟩,, of BCC laths. This is a commonly accepted view (e.g. Schastlivtsev et al., 1999) which attributes to lath martensite two “pseudo-single crystal” slip families, close to ⟨110⟩, and ⟨112⟩, that can activate in a FCC lattice. In this view, also referred to in Mine et al. (2013), the presence and the potential role of interlath retained austenite is ignored.

However, the strong difference in CRSS observed in Mine et al. (2013) may be due to the presence and activity of two different phases in lath martensite: BCC laths with FCC interlath retained austenite. The latter is known to be much weaker than highly dislocated BCC phase. Furthermore, some fractography views reported in Mine et al. (2013) (cf. Fig. 9d in Mine et al., 2013) suggest that ductile shear fracture can occur when lath habit planes are oriented ca. 45° with respect to the tensile axis, i.e. when shear occurs along the BCC–FCC interface. This observation is consistent with Maresca et al. (2014), and therefore calls for an in-depth analysis. Indeed, Maresca et al. (2014) lacks an experimental validation, which is provided here.

This paper aims to assess, based on the experimental results of Mine et al. (2013), the hypothesis proposed in Maresca et al. (2014). We investigate the role played by the hierarchical crystallographic structure of martensite, combined with the presence of very thin interlath austenite films, on the orientation dependent mechanical behaviour of lath martensite, as indicated by the experiments of Mine et al. (2013). To this purpose, a computational framework at the scale of martensite subgrains has been developed, incorporating the mechanical behaviour of martensitic laths through an underlying lamella model. At the scale of the lamella model, the crystallography of the BCC lath and FCC interlath retained austenite is included and modelled using a crystal plasticity approach (Bronkhorst et al., 1992). This two-scale model is used to simulate the deformation behaviour of two martensitic samples of different crystallography, as presented in Mine et al. (2013). The comparison of the simulation results with the experimental data (Mine et al., 2013) reveals the possible contribution of the interlath retained austenite to the deformation behaviour of lath martensite.

The paper is organised as follows. First, in Section 2 a brief summary is given of the existing experimental evidence on the morphology and crystallography of lath martensite and interlath retained austenite. Then, the modelling approach and the model setup are presented in Section 3 and 4, respectively. In Section 5 simulation results are presented and confronted with the experiments by Mine et al. (2013). The paper ends with a discussion and conclusions.

As stated above, lath martensite is in general a mixture of BCC laths and FCC retained austenite films. However, the presence of FCC films is usually neglected. It is shown that by accounting for the presence of BCC and a small volume fraction
(5%) of FCC in lath martensite, the experimental results of Mine et al. (2013) are qualitatively well captured, in particular the flow behaviour, the roughness and slip patterns. In addition, we show in Appendix B that, when the FCC phase is neglected and lath martensite is modelled as a collection of BCC crystals only, the observed experimental flow curves are not captured.

The following notation shall be used: \(a\), \(b\), \(c\) and \(d\) denote scalars, vectors, second order tensors and fourth order tensors respectively. Symbol \(\mathbf{T}\) denotes transposition. Single and double contractions are denoted by “\(\cdot\)“ and “\(:\)”, respectively, with \(\mathbf{A}:\mathbf{B} = \text{tr}(\mathbf{A}\cdot\mathbf{B})\), \(\text{tr}\) being the trace operator. Tensor (or dyadic) product between two vectors \(a\) and \(b\) is denoted \(a\otimes b\). The symbol “\(\times\)” indicates the cross product. The time derivative of scalars and tensors is indicated by a superimposed dot, e.g. \(\dot{a}\).

2. Lath martensite

2.1. Crystallography and morphology of lath martensite

Recent experimental EBSD and TEM investigations (Morito et al., 2003, 2006) on low carbon (0–0.6 wt%), low alloy lath martensite in martensitic steels provide detailed information on the crystallography and morphology of lath martensite. Laths can be considered as highly dislocated BCC crystals. They are related to the prior FCC austenite lattice by an approximately Kurdjumov–Sachs (KS) orientation relationship (Nambu et al., 2013).

As described e.g. in Morito et al. (2006) (see also Fig. 1), laths formed in the same prior austenite crystal are grouped together into subgrains, i.e. 4 crystallographic packets (sets of laths sharing the same habit plane). A packet consists of 3 blocks, each subdivided into two subblocks (collections of laths having the same long direction). The two subblocks which form a block are 2 KS variants, which are characterised by a small crystallographic misorientation: 10.5°/011\(\alpha\); the experimentally measured misorientation angle is even lower (below 5°, Morito et al., 2003). The average crystallography of the two KS variants in each block corresponds to a variant of the Nishiyama-Wassermann (NW) orientation relationship. A one-to-one correspondence can be determined between a low-angle misoriented KS variant pair in a crystallographic packet and a single NW variant, following the notion of Bain axes (e.g. Guo et al., 2004). In Appendix A, Table A1 shows all possible KS variants, while Table A2 shows the related NW variants.

EBSD measurements in Mine et al. (2013) do not allow to clearly distinguish between the two variants of a block. Therefore we will consider the NW orientation relationship for modeling purposes, unless a single KS variant per block is indicated in Mine et al. (2013).\(^1\)

Typical dimensions of blocks in Mine et al. (2013) range from few microns to ca. 10 \(\mu\)m. The thickness of the laths is expected to be of the order of 100–200 nm. In general, the dimensions of crystallographic packets and blocks in lath martensite can vary considerably, depending on the prior austenite grain size (Morito et al., 2005).

2.2. Interlath retained austenite

Thin films of interlath retained austenite can exist along the boundary of each substructural unit of a martensite grain. Their presence has been reported in various low carbon steels (Bhadesia, 1979; Law and Edmonds, 1980; Kim and Thomas, 1981; Rao and Sachdev, 1982; Samuel, 1985; Lee and Su, 1999; Nakagawa and Miyazaki, 1999; Jha and Mishra, 1999; Morito et al., 2011; Baltazar Hernandez et al., 2011; Kim et al., 2012; Nayak et al., 2012; Song et al., 2012). Austenite can be retained at room temperature because of either chemical or mechanical stabilisation. The first phenomenon is due to the alloying composition, while mechanical stabilisation occurs due to the accommodation of the strains involved into the austenite to martensite transformation.

Few data in the literature provide indications on the thickness of interlath retained austenite. Recent investigations on low alloyed martensite (0.2 C, 1.98 Mn martensitic steel) deduce a thickness between 3 and 10 nm (Morito et al., 2011). In quenched martensite, the thickness of retained austenite can be above 20 nm (Kim et al., 2012). The interlath films can

\(^1\) It has been verified that the conclusions do not change qualitatively if, instead of NW, one of the two KS variants is used to model each block.
have a non-constant thickness and be interrupted; however we have shown in Maresca et al. (2014) that also in this case the FCC layers can preserve a significant effect on the mechanical behaviour of a block.

3. Modelling approach

3.1. General framework

Experimental evidence on the substructure of lath martensite, as shortly summarised in the previous section, calls for a multi-scale modelling approach as sketched in Fig. 2. Following the experiments of Mine et al. (2013), the sample scale, subsequently called mesoscale, consists of several martensitic blocks. As explained earlier, at the fine scale each of the blocks consists of laths with interlath retained austenite. Since the direct resolution of the fine laths at the scale of blocks is practically infeasible, the behaviour of the mesoscale material points is obtained through homogenisation, using an underlying lamella model. The lamella model represents the behaviour of a BCC lath with the FCC interlath retained austenite. At the scale of the lamella model, the respective crystallography of the two phases and the resulting elastic and plastic anisotropy are modelled through a crystal plasticity approach.

Next, the lamella model is described, followed by a brief summary of the crystal plasticity formulation.

3.2. Lamella model

We formulate a lamella model which represents a martensite block of laths as an infinite laminate of BCC and FCC phases. The equations of the lamella model are given by

\[
F^M = f^F F^F + f^B F^B, \quad (1)
\]

\[
P^M = f^F P^F + f^B P^B, \quad (2)
\]

\[
P^B \cdot n = P^F \cdot n, \quad (3)
\]

\[
F^B \cdot (I - n \otimes n) = F^F \cdot (I - n \otimes n). \quad (4)
\]

Eqs. (1) and (2) express the mesoscale deformation gradient tensor \(F^M\) and the mesoscale first Piola–Kirchhoff stress \(P^M\) as the volume average of the related phase quantities, with \(f^F\) and \(f^B\) the phase volume fractions; \(F\) and \(B\) indicate FCC and BCC phase, respectively. Eqs. (3) and (4) are the equilibrium and compatibility conditions at an interface, respectively; \(n\) is the interface normal and \(I\) is the second-order identity tensor.

The outcome of this model is equivalent to a fully resolved finite element model of a bicrystal laminate as considered in Maresca et al. (2014).

3.3. Crystal plasticity framework

For the solution of the lamella rule of mixtures, classical crystal plasticity (cf. Bronkhorst et al., 1992) is adopted for each phase. In this first-order continuum approach, the effect of dislocation glide on slip systems is modelled in an average sense, while higher-order effects due to e.g. dislocation pile-ups are disregarded. The typical dimensions of the crystals considered here range from 5 to 200 nm. The possible size effects due to these small features, however, are not included in the present model. Moreover, it is assumed that there are enough dislocations to contribute to the dislocation mediated plasticity. Indeed, despite their small sizes, both laths and interlath retained austenite are known to be highly dislocated. Furthermore, the plastic slip in the austenite films occurs primarily on the slip systems which are approximately parallel to the FCC austenite–BCC lath interface, due to the orientation relationship (cf. Maresca et al., 2014). The in-plane dimension of the austenite films is estimated to be of the order of micrometers, thus justifying the continuum modelling approach.
In this section all quantities refer to each single phase separately; hence, the superscripts $F$ and $B$ are omitted here for the sake of simplicity.

Let us consider the deformation gradient of a phase $\mathbf{F} = \nabla \mathbf{y} (\mathbf{x})$, where $\mathbf{y}$ and $\mathbf{x}$ are the positions of a material point in the current and reference configuration, respectively. The total deformation $\mathbf{F}$ can be multiplicatively split into an elastic $\mathbf{F}_e$ and plastic $\mathbf{F}_p$ contribution as follows:

$$
\mathbf{F} = \mathbf{F}_e \cdot \mathbf{F}_p.
$$

The multiplicative split introduces an intermediate configuration distorted by the plastic deformation only (Fig. 3). The elastic deformation, as well as rotations are included in $\mathbf{F}_e$.

Next, the plastic part of the velocity gradient $\mathbf{L}$ is introduced as $\mathbf{L}_p = \mathbf{F}_p \cdot \mathbf{F}_e^{-1}$. In the crystal plasticity setting, the crystallographic decomposition reads

$$
\mathbf{L}_p = \sum_{\alpha = 1}^{n_s} \mathbf{\hat{\gamma}}^\alpha \mathbf{P}_0^\alpha,
$$

where $\mathbf{P}_0^\alpha = \mathbf{s}_0^\alpha \otimes \mathbf{n}_0^\alpha$ is the Schmid tensor of the $\alpha$th slip system, $\mathbf{s}_0^\alpha$ is the slip direction and $\mathbf{n}_0^\alpha$ the slip normal, both defined in the reference configuration, $\mathbf{\hat{\gamma}}^\alpha$ is the plastic slip rate on slip system $\alpha$ and $n_s$ is the number of slip systems in the crystal.

The pull back of the Kirchhoff tensor $\mathbf{\tau}$ to the intermediate configuration gives

$$
\mathbf{\bar{S}} = \mathbf{F}_e^{-1} \cdot \mathbf{\tau} \cdot \mathbf{F}_e^{-T}.
$$

The constitutive relation for $\mathbf{\bar{S}}$ is taken as

$$
\mathbf{\bar{S}} = \mathbf{C} : \mathbf{E}_e,
$$

where $\mathbf{C}$ is the fourth-order elasticity tensor, $\mathbf{E}_e = \frac{1}{2} \left( \mathbf{C}_e - \mathbf{I} \right)$ is the elastic Green-Lagrange strain with $\mathbf{C}_e = \mathbf{F}_e^T \cdot \mathbf{F}_e$ the elastic Cauchy-Green tensor.

The plastic slip rate $\mathbf{\hat{\gamma}}^\alpha$ is determined via the visco-plastic slip law (Hutchinson, 1976)

$$
\mathbf{\hat{\gamma}}^\alpha = \hat{\gamma}_0 \left( \frac{|\mathbf{\tau}^\alpha|}{\mathbf{s}^\alpha} \right)^m \text{sign}(\mathbf{\tau}^\alpha),
$$

where $\hat{\gamma}_0$ is a reference slip rate and $m$ is a strain rate sensitivity parameter; $\mathbf{\tau}^\alpha$ is the shear stress resolved on the $\alpha$th slip system:

$$
\mathbf{\tau}^\alpha = \left( \mathbf{C} \cdot \mathbf{\bar{S}} \right)^T : \mathbf{P}_0^\alpha.
$$

The current slip resistance $\mathbf{s}^\alpha$ follows the evolution law

$$
\mathbf{s}^\alpha = \sum_{\beta = 1}^{n_s} h^\alpha \beta |\mathbf{\dot{\gamma}}^\beta|,
$$

where $h^\alpha \beta$ is a hardening matrix, which takes the form

$$
h^\alpha \beta = h_0 \left( 1 - \frac{s^\alpha}{s_{\infty}} \right)^a q^\alpha \beta,
$$

with $q^\alpha \beta$ a matrix in which elements equal 1 on the diagonal and $q_n$ off diagonal ($q_n$ is the ratio of the latent hardening with respect to the self-hardening for non-coplanar slip systems); $h_0$, $s_{\infty}$ and $a$ are material parameters.

---

**Fig. 3.** Multiplicative split of the deformation gradient. Blue lines indicate schematically a slip system in each configuration. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)
The Schmid’s law (10) is violated in BCC crystals. Therefore, non-Schmid effects in the BCC phase are included (e.g. Dao and Asaro, 1993; Yalçinkaya et al., 2008) by redefining the resolved shear stress as

\[ \tau^\alpha = (C_e \cdot \tilde{S})^T : P^\alpha_{0n}, \]  

where \( P^\alpha_{0n} = P^\alpha_{0n} + \eta^\alpha \), with \( \eta^\alpha \) defined by Yalçinkaya et al. (2008):

\[ \eta^\alpha = \eta_{ss} n_{0s} \otimes n_{0s} + \eta_{nn} n_{0n} \otimes n_{0n} + \eta_{zz} z_{0} \otimes z_{0} \]  

(no sum on \( \alpha \)).

In (14), \( \eta_{ss}, \eta_{nn} \) and \( \eta_{zz} \) are three non-Schmid parameters, while \( z_{0} = n_{0s} \times n_{0n} \).

3.4. Numerical implementation

The computational framework as presented above involves two levels of analysis: the lath martensite specimen is discretised with 3D tri-linear brick finite elements. To each element within the block the average spatial orientation of the laths is assigned, and the corresponding lamella model is solved at each integration point. Within the solution of the model, the crystal plasticity algorithm is invoked for each phase. The whole framework has been implemented in a user-defined element subroutine in a commercial FE code. A Total Lagrange procedure is used to account for finite deformations. Newton–Raphson procedures are used both for the solution of the lamella model at each mesoscale integration point and for the solution of the non-linear crystal plasticity slip laws in each phase. A fully implicit backward-Euler scheme is adopted for the time discretization of the constitutive equations.

Computational efficiency was not the aim of this work, which focuses on gaining physical insight instead. For this reason, the routines were not optimized for parallelization and the simulations were done on a single core.

4. Simulation setup

4.1. Mesoscale geometry and crystallography

The model is assessed on specimens MP1 and MP2 of Mine et al. (2013). The EBSD measurements from Mine et al. (2013) showing the crystallographic orientations of the BCC phase are reported in Fig. 4.

According to these EBSD data, two geometrical models have been created, hereafter referred to as configuration MP1 and configuration MP2, respectively (see Fig. 5).

The in-plane dimensions of the models are \( H = 20 \, \mu m, \, L_1 = 32.14 \, \mu m, \, L_2 = 26.32 \, \mu m \). Thus, only a fraction of the specimen with 50 \( \mu m \) gauge length is modelled.

![Fig. 4. EBSD maps in the undeformed configuration of specimens MP1 (a) and MP2 (b). Reprinted from Mine et al. (2013) with permission from Elsevier.](image)

![Fig. 5. Model geometry and finite element mesh for specimen MP1 (a) and MP2 (b), with variants and crystallographic packets (CP) indicated.](image)
For both configurations, the out-of-plane dimension is $T = 20 \, \mu m$. Since the morphology and the crystallography of the samples is not known in the out-of-plane direction, it has been assumed constant through the thickness. As far as configuration MP2 is concerned, the assumption of constant out-of-plane morphology seems not far from reality, by considering Fig. 2 in Mine et al. (2013) and by noticing that the lath habit plane in CP4 is approximately perpendicular to the specimen top surface. The situation is less clear in case of configuration MP1. However, also in this case (Fig. 2 in Mine et al., 2013) the typical size of the blocks seems to be comparable with the specimen thickness size.

Fig. 5 also shows the KS variants measured experimentally by Mine et al. (2013) in each block, together with the NW variants used in our models, see Appendix A for the crystallographic definition of these variants. Furthermore, where the analysis in Mine et al. (2013) indicates a single KS variant (V10 in MP1 and V5 in MP2, cf. Fig. 4), only the measured KS variant has been assigned to the block.

4.2. Finite element model and boundary conditions

The considered parts of the specimens have been discretized by 3D tri-linear brick finite elements. The average in-plane FE size is around 0.5 $\mu m^2$. For both configurations MP1 and MP2, the FE mesh is shown in Fig. 5. Four elements are used through the thickness, since the variations of the strain field in that direction are small. For both the in-plane and through the thickness directions we have performed a mesh refinement study. This study revealed that, although the selected mesh is relatively coarse, the convergence of the results is satisfactory.

In both configurations, boundary conditions are applied such that the loading on a central section of dogbone specimens could be mimicked, Fig. 6. The bottom and back edges of the lateral faces (dashed in Fig. 6) of the modelled material volume were constrained in $y$- and $z$-directions, respectively, while leaving other degrees of freedom unconstrained to allow for free transverse contraction and expansion. This also ensures that no relative shear along $y$- and $z$-directions takes place, which is expected to be impeded by the aligned clamps. One point of the model is also fixed to eliminate rigid body rotations and translations.

The two faces of the model which are perpendicular to the $X$ direction represent virtual cross-sections of the real specimen away from the clamps. For this reason, displacement along $X$ direction (i.e. tensile axis) is prescribed in an average sense, i.e. for the left face

$$\langle u_X \rangle = \frac{1}{\Omega_L} \int_{\Omega_L} u_X \, d\Omega = 0$$

(15)

In (15) $\Omega_L$ is the area of the left face. Similarly, on the right face the average $X$-displacement reads

$$\langle u_X \rangle = \frac{1}{\Omega_R} \int_{\Omega_R} u_X \, d\Omega = \Pi_X,$$

(16)

where $\Pi_X$ is such that $\varepsilon_{XX} = (d/dt)(\partial \Pi_X / \partial X) = 0.01 \, s^{-1}$; $\Omega_R$ is the area of the right face.

4.3. Material parameters of single phases

We will consider an FCC volume fraction $f_f = 4.76\%$, which for example may correspond to a scenario in which laths are 100 nm thick and interlath retained austenite is 5 nm thick.

The FCC phase is characterised by the standard $(111)_f$ family slip systems. For the BCC phase, the $(110)_t$ slip system family has been assumed to be active at room temperature (e.g. Gröger et al., 2008; Caillard, 2010).

The parameter identification procedure is detailed next. First, the anisotropic elastic constants in the FCC and BCC phases have been determined based on data from the literature (Turteltaub and Suiker, 2005), where they were determined from indentation experiments (Furnémont et al., 2002). For the BCC martensite, we identified the elastic constants by following the same procedure as proposed in Turteltaub and Suiker (2005). Next, the initial slip resistance $\tau_0$ for the slip systems in the two phases has been determined while adopting a strain rate sensitivity $m = 0.10$ and a reference slip rate of $\dot{\gamma}_0 = 0.01 \, s^{-1}$. The non-Schmid parameters for the BCC phase have been taken from the literature (Yalçinkaya et al., 2008). The initial slip resistance $\tau_0$ of the FCC phase was first identified on the stress–strain response of MP2 configuration, which is much more

Fig. 6. Boundary conditions applied on both configurations MP1 and MP2. (For interpretation of this figure, the reader is referred to the color web version of this paper.)
sensitive to this value than configuration MP1, by assuming a first guess of the initial slip resistance in the BCC phase $\tau_0 = 530$ MPa. This value has been chosen close to the value estimated in Mine et al. (2013) as the critical resolved shear stress (CRSS) of $f_{112}g_\alpha$ slip systems. After fitting the stress–strain response of MP2, the $\tau_0$ for the BCC phase has been corrected such that the stress–strain response of configuration MP1 matches. The process has been iterated a couple of times until both stress–strain responses of MP1 and MP2 match. The number of iterations was limited, since the deformation behaviour of configuration MP2 is dominated by the FCC phase in most of the domain, while the deformation of configuration MP1 is mostly dominated by the BCC phase, due to the preferential orientation of the habit planes with respect to the applied tensile loading, as will be shown in the Results section. Therefore the stress–strain response of configuration MP2 is more sensitive to the initial slip resistance of the FCC phase than of the BCC phase, while the opposite situation is encountered in configuration MP1. Finally, the initial hardening rate $h_0$ and the slip resistance saturation value $s_1$ have been matched, while assuming a hardening exponent $a = 1.5$ and a ratio between latent and self hardening $q_{n} = 1.4$.

The identification of these parameters followed the same steps as the identification of the initial slip resistances described above.

The material parameters used in the simulations are listed in Table 1.

### Table 1

<table>
<thead>
<tr>
<th>Material parameter</th>
<th>FCC</th>
<th>BCC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial slip resistance</td>
<td>$\tau_0$</td>
<td>265 MPa</td>
</tr>
<tr>
<td>Slip resistance saturation value</td>
<td>$s_{\text{sat}}$</td>
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</tr>
<tr>
<td>Initial hardening rate</td>
<td>$h_0$</td>
<td>250 MPa</td>
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<tr>
<td>Reference slip rate</td>
<td>$\tau_\text{ref}$</td>
<td>0.01</td>
</tr>
<tr>
<td>Strain rate sensitivity</td>
<td>$m$</td>
<td>0.10</td>
</tr>
<tr>
<td>Hardening exponent</td>
<td>$a$</td>
<td>1.5</td>
</tr>
<tr>
<td>Ratio latent/self hardening</td>
<td>$q_{n}$</td>
<td>1.4</td>
</tr>
<tr>
<td>Non-Schmid parameter $\eta_{ss}$</td>
<td>0.0544</td>
<td></td>
</tr>
<tr>
<td>Non-Schmid parameter $\eta_{nn}/C_0$</td>
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<td></td>
</tr>
<tr>
<td>Non-Schmid parameter $\eta_{zz}/C_0$</td>
<td>-0.0267</td>
<td></td>
</tr>
<tr>
<td>Elastic constant $C_{11}$</td>
<td>268.5 GPa</td>
<td>349 GPa</td>
</tr>
<tr>
<td>Elastic constant $C_{12}$</td>
<td>156 GPa</td>
<td>202.5 GPa</td>
</tr>
<tr>
<td>Elastic constant $C_{44}$</td>
<td>136 GPa</td>
<td>176.5 GPa</td>
</tr>
<tr>
<td>Elastic constant $C_{12}$</td>
<td>156 GPa</td>
<td>202.5 GPa</td>
</tr>
<tr>
<td>Elastic constant $C_{44}$</td>
<td>136 GPa</td>
<td>176.5 GPa</td>
</tr>
</tbody>
</table>

Fig. 7. Flow curves of configurations MP1 and MP2 vs experimental results from Mine et al. (2013). (For interpretation of this figure, the reader is referred to the color web version of this paper.)
limitations in the experimental accuracy for small strains. Indeed the elastic modulus $C_{11}$ that would correspond with the experimental data points, raises up to 800 GPa, which seems unrealistic. Moreover, we have verified that the conclusions are not affected qualitatively by the choice of different elastic constants.

5.2. Slip activity

The analysis of the slip activity in the single phases for specimens MP1 and MP2 gives insight in the different flow behaviour obtained for the two configurations. Figs. 8 and 9 show the total slip in FCC and BCC phases, respectively, for both samples at 1.0% applied axial strain.

Considering the total slip in the FCC phase for configuration MP2 (Fig. 8(b)), two distinct areas of slip can be recognised, corresponding to the crystallographic packets present in the specimen. The most intense slip activity is in CP4 (V19/V22, V20/V23, V21/V24), since there the FCC phase is most favourably oriented for accommodating deformation by shear. This corresponds qualitatively well with the experimental observations by Mine et al. (2013), who have also observed the maximum slip activity in this crystallographic packet, in particular in the right-side block V20/V23. Compared to CP4, the other blocks (belonging to CP1 – V1/V4, V5 - and CP2 – V7/V10, V8/V11) accommodate less slip. The BCC phase hardly contributes to the plastic deformation; its total slip activity being well below 2% in all blocks, not above 0.2% in most of the specimen, Fig. 9(b). In essence, in 76% of the specimen domain the average total slip activity in FCC is around 40% and the total slip activity in BCC is below 0.2%. This means an FCC/BCC activity ratio of 200, for most of the specimen domain.

For the MP1 sample, intense slip activity in FCC phase is registered (the same order of magnitude as in CP4 for MP2) in a much smaller domain, occupied by V20/23 and V21/24, see Fig. 8(a). Most blocks have a total slip activity in the FCC phase below 10% (V13/16 and V15/18), while the total slip activity in the BCC phase reaches peaks above 4% (in V15/18) and shows average values of 1.0% in a large domain (the whole specimen except V21/24), Fig. 9(a). This implies that the majority of the MP1 volume has an average total plastic slip activity in FCC around 10%, while the total slip activity in BCC is around 1.0%. This results in a FCC/BCC activity ratio of 10, for the majority (67%) of the specimen domain, i.e. around 20 times lower compared to specimen MP2.

This observation explains the difference in yielding response between MP1 and MP2 as shown in Fig. 7. The deformation of specimen MP2 is mostly dominated by the slip activity in the FCC phase, therefore the yield point is relatively low and also hardening is governed by the moderate hardening parameters of the FCC phase. On the other hand, the BCC phase plays a more important role in MP1, as discussed above. This leads to a higher yielding point compared to MP2, and a more pronounced influence of the BCC phase on the overall hardening behaviour.

![Fig. 8. Total plastic slip in FCC phase for configurations MP1 (a) and MP2 (b), 1.0% applied axial strain.](image)

![Fig. 9. Total plastic slip in BCC phase for configurations MP1 (a) and MP2 (b), at 1.0% applied axial strain.](image)
Finally, it should be remarked that this result is not just dependent on the orientation of FCC slip systems with respect to the loading. It is rather due to the presence of blocks whose BCC–FCC interfaces are favourably oriented with respect to loading, promoting localised shear deformation along the interface, being carried by the FCC slip systems parallel to the interface.

5.3. Roughness pattern

Fig. 10(b) shows the roughness pattern of configuration MP2 at 1.0% strain, normalized with respect to the maximum height difference on the surface. Comparisons with Fig. 10(a), showing the experimental measurements by Mine et al. (2013), indicate that the qualitative pattern is adequately captured, with bands of increased roughness forming at $45^\circ$ with respect to the loading direction. Note, that only a qualitative comparison of roughness patterns is possible, since absolute values of the roughness depend strongly on the through thickness morphology, crystallography and constraining conditions, which are reproduced here in a rather approximated manner, since they are essentially unknown.

6. Discussion

Results of the simulations of martensite specimens show that, by assuming the presence of a small volume fraction of retained FCC austenite layers along BCC lath boundaries, the main qualitative features of the lath martensite mechanical behaviour experimentally observed in Mine et al. (2013), are captured.

In particular, when lath habit planes are oriented ca. $45^\circ$ with respect to the uniaxial loading direction, shear localisation occurs in the FCC phase, which accommodates most deformation. Indeed, a small volume fraction (about 5%) of interlath retained austenite may trigger the apparent large deformation behaviour of the phase mixture, which is generally still called martensite.

The presence of interlath retained austenite, combined with the crystallography of the laths, can therefore be a plausible explanation of the orientation dependent yielding and hardening behaviour of “lath martensite” (which is the main phase), as experimentally observed in Mine et al. (2013). By fixing the critical resolved shear stress (CRSS) and hardening parameters of BCC and FCC phases, and by assuming relatively low hardening of the FCC phase, it is possible to recover the yield stress and the hardening behaviour for both specimens MP1 and MP2. The lower yield stress for the specimen MP2 can be explained by the localisation of deformation in the blocks favourably oriented for shearing; MP1 has a smaller volume fraction of the favourably oriented blocks, thus showing a higher yield stress. Furthermore, after localised shear is activated in MP2, almost no hardening is observed, since deformation can be easily accommodated by the FCC phase in the favourably oriented blocks, without a substantial role for the BCC phase; in MP1 the BCC phase contributes significantly and flow curves show hardening.

Note, that the localised shearing mechanism is not merely due to the orientation of the FCC phase in the material with respect to loading: the FCC phase has the same orientation throughout the whole specimen (since all martensitic blocks come from the same parent FCC grain). It is rather the relative orientation of the BCC–FCC interface (or $\gamma$–$\alpha'$ habit plane) with respect to the loading that plays the major role: only the FCC slip systems parallel to the interface contribute to the plastic deformation, while the other slip systems remain largely inactive.

Literature on mechanical behaviour of lath martensite (e.g. Schastlivtsev et al., 1999; Michiuchi et al., 2009) usually neglects any role of interlath retained austenite on deformation. Instead, two pseudo-single crystal slip planes in lath martensite are assumed as being active at room temperature, i.e. $(110)_{\alpha'}$ (the one considered in our study for the BCC phase) and $(112)_{\alpha'}$. We have verified, see Appendix B, that when it is assumed that interlath retained austenite does not play any role and that the BCC laths deform according to these two slip systems, then a different yielding and hardening behaviour of the two samples results, whereby the observed experimental curves cannot be recovered. If only one of the two slip systems is considered, while still neglecting the presence of interlath retained austenite, the orientation effect cannot be captured either, see Appendix B. Therefore, only the presence of interlath retained austenite seems to explain both the apparent slip traces occurring along lath habit planes and the
observed orientation dependent behaviour of lath martensite (e.g. Mine et al., 2013; Ghassemi-Armaki et al., 2013). Moreover, interlath retained austenite may well contribute to the observed ductile fracture behaviour, e.g. in specimen MP2 (Mine et al., 2013).

Austenite layers are used to improve toughness and ductility of martensite in the new generation of advanced high strength steels (AHSS), recently presented in the literature (De Moor et al., 2008; Raabe et al., 2013). One example is the quenching and partitioning (Q&P) processing, where austenite layers thicker than those considered here are promoted. An even more recent example is the "reversed" austenite obtained in maraging steels (Raabe et al., 2013). After processing, the interlath austenite films reveal, at least partially, a KS orientation relationship with the adjacent BCC laths. Furthermore, their thickness (5–15 nm) is of the same order of magnitude as that of the interlath retained austenite layers considered in the present work.

The present simulations reproduce the experimental flow curves quantitatively well, while results on slip activity and roughening remain qualitative. This is due to the fact that the two latter phenomena strongly depend on the detailed morphology and crystallography, which is not sufficiently accessible due to experimental limitations and due to the fact that the through-thickness information can be obtained by destructive experimental methods only. A more detailed, quantitative investigation based on accurate experimental tests will be required to improve on this.

Furthermore, our work does not account for possible austenite to martensite phase transformation during deformation. Most work on TRIP phenomena considers chemically retained islands of austenite which loose their stability at relatively low strains. However, interlath retained austenite is supposed to be both chemically and mechanically stabilised, due to the high strain induced in austenite by the transformation strain of the laths. Therefore, the onset of transformation should not occur under the same conditions as it would be in a chemically stabilised austenite. Therefore, further work may account for phase transformations, considering the role played by the mechanical stabilisation. Consequently, internal stresses generated by the transformation could be taken into account. Moreover, the deformability of lath martensite is expected to change if interlath austenite transforms into hard, interlath martensite.

The crystal plasticity model does not include damage. The present results suggest that FCC layers with a high value of localised shear may be a preferential location for the onset of damage. For example, in MP2 samples fracture occurs in the blocks where both our model and experiments (Mine et al., 2013) show the most intense slip activity. The presence of damage in austenite could amplify the apparent deformation of lath martensite, which is a mixture of BCC and FCC phases, by weakening the FCC layers. This is the subject of future work.

7. Conclusions

The main results are summarised in the following.

1. By accounting for the presence of a small volume fraction of interlath retained austenite (5%), it is possible to model and reproduce numerically the main features of the experimentally observed deformation behaviour of lath martensite, which is a mixture of BCC and FCC phases. Flow curves can be quantitatively recovered, while slip activity and roughening pattern are captured qualitatively, since their detailed description depends on unresolved fine morphological and crystallographic features.

2. The presence of interlath retained austenite can be a plausible explanation of the observed apparent large deformation behaviour and ductility of the BCC–FCC mixture (usually considered as lath martensite only without interlath austenite films) reported in the literature. As long as there are enough carriers for plasticity, a small quantity of interlath retained austenite can enhance the deformation of lath martensite. When interlath retained austenite films are favourably oriented with respect to the loading direction, the same deformation level is obtained at lower stress values, with shear localisation occurring in interlath films. The main, new contribution of the present paper is the validation of the model of lath martensite with interlath retained austenite with respect to experimental data.

3. If the presence of interlath austenite is neglected, classical first order crystal plasticity modeling of BCC laths is not capable to capture the experimentally observed flow curves.

Our results further suggest that the presence of interlath retained austenite can be a plausible explanation of the experimentally observed orientation dependent behaviour of lath martensite, which is a mixture of FCC austenite films and BCC laths. A detailed experimental–numerical study will be performed in the future to obtain a more quantitative analysis of the local deformation behaviour and stress–strain response of lath martensite. The influence of damage on lath martensite mechanics will also be investigated.

Acknowledgments

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Appendix A. List of variants for KS and NW orientation relationships

Table A1 lists all possible variants of KS orientation relationship.
Table A2 lists all possible variants of NW orientation relationship.
Table A1
24 variants of KS OR, grouped by crystallographic packets (see Morito et al., 2003).

<table>
<thead>
<tr>
<th>NW variant</th>
<th>Parallel plane</th>
<th>Parallel direction</th>
<th>KS variants of same Bain group</th>
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</thead>
<tbody>
<tr>
<td>NW1</td>
<td>(111),/{011}_l</td>
<td>{101}_l/{100}_l</td>
<td>V1–V4</td>
</tr>
<tr>
<td>NW2</td>
<td>(111),/{011}_l</td>
<td>{101}_l/{100}_l</td>
<td>V3–V6</td>
</tr>
<tr>
<td>NW3</td>
<td>(111),/{011}_l</td>
<td>{011}_l/{100}_l</td>
<td>V2–V5</td>
</tr>
<tr>
<td>NW4</td>
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<td>NW5</td>
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<td>V15–V18</td>
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<td>NW6</td>
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<td>NW12</td>
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Table A2
The 12 variants of the NW OR and the KS variants of the same Bain group (see Guo et al., 2004).

<table>
<thead>
<tr>
<th>NW variant</th>
<th>Parallel plane</th>
<th>Parallel direction</th>
<th>KS variants of same Bain group</th>
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<td>(111),/{011}_l</td>
<td>{110}_l/{100}_l</td>
<td>V20–V23</td>
</tr>
</tbody>
</table>

Appendix B. Response of models not accounting for interlath retained austenite

In order to further support the interpretation of the role played by interlath retained austenite in the deformation behaviour of lath martensite (which is a mixture of BCC laths and FCC interlath austenite films), we consider the response of configurations MP1 and MP2 (cf. Section 4.2) in case no FCC phase is present and plastic flow is completely due to the BCC laths. None of the crystallographically possible options can reproduce the flow curves measured by Mine et al. (2013), unless slip within the interlath retained austenite films is included into the model.

B.1. “Classical” lath martensite framework

Works devoted to the mechanical behaviour of lath martensite (e.g. Schastlivtsev et al., 1999; Mine et al., 2013) neglect the presence and role of interlath retained austenite and consider the presence of two pseudo-single crystal slip families:

1. \{110\}_l/\{111\}_l, also called “in-lath-plane” slip system family;
2. \{112\}_l/\{111\}_l, also named “out-of-lath-plane” slip system family.

Note, that for lath martensite \{110\}_l/\{111\}_l and in case of KS orientation relationship \{111\}_l/\{011\}_l. This means that some \{110\}_l slip systems act on the same planes as FCC slip systems parallel to BCC–FCC interface in our model. However, they are spread through the laths and they are not localised in thin films. We refer to this model as the “classical” lath martensite framework.
We reconsider configurations MP1 and MP2 presented in Section 4.2. The BCC laths are assigned the same orientations as specified in Fig. 5. The BCC slip systems of both \( \{110\} \) \( \langle \alpha \rangle \) and \( \{112\} \) \( \langle \alpha \rangle \) families are included as discussed above. The presence of FCC interlath austenite is neglected.

New material parameters are identified such that experiments of specimen MP2 match. For \( \{110\} \) \( \langle \alpha \rangle \) slip systems, \( \tau_0 = 370 \) MPa (i.e. similar value as reported in Mine et al., 2013), \( s_1 = 0.7 \) GPa and \( h_0 = 1.2 \) GPa, the other parameters being equal to those listed in Table 1 for the BCC phase. For \( \{112\} \) \( \langle \alpha \rangle \) slip systems, \( \tau_0 = 550 \) MPa (also in this case, a value similar as reported in Mine et al., 2013), \( s_\infty = 2.0 \) GPa and \( h_0 = 3.0 \) GPa. Non-Schmid effects for \( \{112\} \) \( \langle \alpha \rangle \) slip systems are also included, with the same non-Schmid parameters as those considered for \( \{110\} \) \( \langle \alpha \rangle \). The remaining parameters are those listed in Table 1 for the BCC phase. The specimen MP1 is modelled with the same material parameters as MP2.

Fig. B1 shows the resulting response of configurations MP1 and MP2 compared to experiments of Mine et al. (2013). From Fig. B1 it can be concluded that if the presence of both \( \{110\} \) \( \langle \alpha \rangle \) and \( \{112\} \) \( \langle \alpha \rangle \) BCC slip families are included, only small differences in yielding response of the two samples are captured. Moreover, the difference is opposite to what the experiments in Mine et al. (2013) show, i.e. MP1 is weaker than MP2.

B.2. BCC with a single slip family active and no interlath FCC films

Next, we consider the case where interlath retained austenite is absent (or plays no role), and just one slip system family is active in the BCC laths. The slip families which are active at room temperature for BCC may be either \( \{112\} \) \( \langle \alpha \rangle \) (e.g. Seeger, 2001; Yalçinkaya et al., 2008) or \( \{110\} \) \( \langle \alpha \rangle \) (e.g. Gröger et al., 2008; Caillard, 2010). For slip system family \( \{110\} \) \( \langle \alpha \rangle \) we consider the parameters mentioned in the previous section. For \( \{112\} \) \( \langle \alpha \rangle \) we consider \( \tau_0 = 360 \) MPa, \( s_\infty = 1.0 \) GPa and \( h_0 = 1.5 \) GPa. In both cases, non-Schmid effects are accounted for. Note that results do not deviate visibly if non-Schmid effects are neglected.

\(^2\) In case non-Schmid effects are neglected for \( \{112\} \) \( \langle \alpha \rangle \) slip systems, results do not visibly deviate from those where non-Schmid effects are considered.
References


