Mechanics of Materials 92 (2016) 198–210

Contents lists available at ScienceDirect

Mechanics of Materials

journal homepage: www.elsevier.com/locate/mechmat

# Reduced crystal plasticity for materials with constrained slip activity

F. Maresca[a,b,*], V.G. Kouznetsova[a], M.G.D. Geers[a]

[a] Department of Mechanical Engineering, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, the Netherlands
[b] Materials innovation institute M2i, P.O. Box 5008, 2600 GA Delft, The Netherlands

ARTICLE INFO

*Article history:*
Received 19 May 2015
Revised 9 September 2015
Available online 26 September 2015

*Keywords:*
Anisotropic plasticity
Crystal plasticity
Finite deformations
Laminates
Lath martensite
Dual phase steels

ABSTRACT

In a number of materials, plasticity occurs along preferential directions or slip systems, while other directions barely contribute to deformation. This can occur due to the specific crystalline nature of the materials (e.g. in polymers) or due to the morphology of the crystalline material itself, like in metal laminates. In the latter case, when the layers are very thin, the surrounding material acts as a constraint and only preferential slip directions are activated. This observation suggests the reduction of the underlying full crystal plasticity model within those regions to a more computationally efficient model which still retains the main deformation mechanism, i.e. plasticity occuring along a few slip systems only. In this paper we propose such a reduced crystal plasticity model in a finite deformation setting. In the limit of either no active slip system or five linearly independent slip systems, the model reduces to isotropic plasticity and standard crystal plasticity, respectively. The model is validated on a specific case, i.e. lath martensite microstructures consisting of alternating crystalline layers of martensite and austenite. The characteristic material behaviour (i.e. stress-strain response and slip activity on the most active slip systems) is correctly reproduced by the reduced model at a significantly lower computational cost compared to a fully resolved crystal plasticity model.



## 1. Introduction

A broad class of materials, like metals and semi-crystalline polymers, exhibit plastic deformation along preferential directions. Crystal plasticity modelling (e.g. Peirce et al., 1982; Bronkhorst et al., 1992) is commonly used to describe the anisotropic plastic response of materials as a function of their crystalline structure. Most models have been extended to finite strains, and they are widely used to model texture evolution, slip activity, roughening, phase transformation and other orientation dependent phenomena in crystalline materials (Roters et al., 2010).

In some cases, due to internal constraining conditions, e.g. the low symmetry or specific structure of the crystals, deformation is governed by plastic slip on a limited number of slip systems. One example can be found in the field of semi-crystalline polymers, where certain inextensible directions are present due to the polymer chain orientations resulting in crystals that lack five independent slip systems (Parks and Ahzi, 1990; van Dommelen et al., 2000). For this case, finite element formulations in the large deformation setting have been proposed, which account for extra kinematical constraints besides incompressibility (e.g. van Dommelen et al., 2000), yet not in a reduced form as proposed here.

Other examples can be found in high strength steels, where some microstructures are characterised by alternate layers of stiffer and softer phases. An example is lath martensite (Kim and Thomas, 1981; Morito et al., 2003), also within the broader context of TRIP maraging steels (Raabe et al., 2013; Wang et al., 2014) and quenched and partitioned (Q&P)

* Corresponding author.
*E-mail address:* f.maresca@tue.nl (F. Maresca).

http://dx.doi.org/10.1016/j.mechmat.2015.09.011

steels (De Moor et al., 2008), as well as bainite or nanobainite (Bhadeshia, 2013). In these cases, the lamellar structure consists of harder body centered cubic (BCC) crystals and softer face centered cubic (FCC) austenite layers. The BCC-FCC layers are generally related by an orientation relationship, which forces the interface between the two phases to be approximately parallel to three slip systems of the $\{111\}_\gamma$ family. The specific crystallographic relationship and the constraining effect of the BCC phase on the austenite induces that only 3 out of the 12 slip systems in the FCC phase carry most of the plastic deformation (Maresca et al., 2014a); plasticity along other directions still occurs, but to a minor extent only.

In this paper, a reduced crystal plasticity model is proposed to account for a limited number of active slip systems, together with some plasticity along the other spatial directions. In this reduced model, the contribution of the most active slip systems is explicitly accounted for within a standard crystal plasticity format (e.g. Peirce et al., 1982; Bronkhorst et al., 1992), while isotropic rate-dependent plasticity (e.g. Belytschko et al., 2009) is used for the remaining spatial directions. This considerably reduces the required computational effort compared to a fully resolved crystal plasticity model. The proposed model is validated using lath martensite microstructures. It is shown that the combination of the reduced crystal plasticity model for the austenite and the isotropic plasticity model for the martensite preserves the main physics of the full crystal plasticity model, while yielding computational speed-ups up to a factor of 10.

The paper is organised as follows. First, in Section 2, the reduced crystal plasticity model is introduced, followed by Section 3 with the constitutive choices. Section 4 shows the finite element implementation. In Section 5, the model is incorporated in a lamella homogenization scheme to mimic the laminated FCC-BCC structure of lath martensite and the results are presented and confronted with the fully resolved simulations from Maresca et al. (2014b), both in terms of material response and computational performance. In Section 6, the lamella model for the martensite with reduced description of the phases is applied in the context of multi-phase (dual phase) steels, and validated against fully resolved simulations on the same microstructures. The paper ends with a discussion and conclusions.

The following notations are used: $a$, $\mathbf{b}$, $\mathbf{C}$ and $\mathbb{D}$ denote scalars, vectors, second-order tensors and fourth-order tensors, respectively. Symbol " $^T$ " denotes transposition. Single and double contractions are denoted by "·" and ":", respectively, with $(\mathbf{A}\cdot\mathbf{B})_{ij} = A_{ik}B_{kj}$ (sum on repeated indices) and $\mathbf{A}:\mathbf{B} = \mathrm{tr}(\mathbf{A}\cdot\mathbf{B})$, "tr" being the trace operator. Tensor (or dyadic) product between two vectors $\mathbf{a}$ and $\mathbf{b}$ is denoted $\mathbf{a}\otimes\mathbf{b}$. The symbol "×" indicates the cross product. The time derivative of scalars and tensors is indicated by a superimposed dot, e.g. $\dot{a}$. The derivative of a second-order tensor $\mathbf{A}$ with respect to a second-order tensor $\mathbf{B}$ is defined as $\frac{\partial \mathbf{A}}{\partial \mathbf{B}} = \frac{\partial A_{ij}}{\partial B_{hk}} \mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_h \otimes \mathbf{e}_k$.

## 2. Reduced crystal plasticity framework

### 2.1. Nomenclature

Table 1 summarizes the list of the main symbols introduced in Section 2.

**Table 1**
List of the main symbols introduced in Section 2.

| | |
|---|---|
| $\mathbf{F}$ | Deformation gradient; |
| $\mathbf{F}_e$ | Elastic part of the deformation gradient; |
| $\mathbf{F}_p$ | Plastic part of the deformation gradient; |
| $\mathcal{B}_r$ | Reference configuration; |
| $\mathcal{B}_0$ | Plastically deformed, intermediate configuration; |
| $\mathcal{B}$ | Current configuration; |
| $\phi_e^*$ | Pull-back operator; |
| $\phi_*^e$ | Push-forward operator; |
| $\mathbf{C}_e$ | Elastic Cauchy-Green tensor; |
| $\mathbf{I}$ | Second order identity tensor; |
| $\mathbb{I}$ | Fourth-order identity tensor; |
| $\mathbf{g}$ | Metric tensor of the current configuration $\mathcal{B}$; |
| $\mathbf{L}$ | Velocity gradient; |
| $\mathbf{L}_e$ | Elastic part of the velocity gradient; |
| $\mathbf{L}_p$ | Plastic part of the velocity gradient; |
| $\bar{\mathbf{L}}_p$ | Pull-back of the plastic part of the velocity gradient to $\mathcal{B}_0$; |
| $\bar{\mathbf{L}}_{p,\gamma}$ | "Slip" contribution to $\bar{\mathbf{L}}_p$; |
| $\bar{\mathbf{L}}_{p,\varepsilon}$ | "Isotropic" contribution to $\bar{\mathbf{L}}_p$; |
| $\mathbf{P}_0^\alpha$ | Schmid tensor in $\mathcal{B}_0$ of the $\alpha$th slip system; |
| $\mathbb{P}_0$ | Fourth order projection operator in $\mathcal{B}_0$; |
| $\mathbb{C}$ | Fourth-order elasticity tensor; |
| $\boldsymbol{\tau}$ | Kirchhoff stress tensor; |
| $\bar{\mathbf{S}}$ | Pull-back of $\boldsymbol{\tau}$ to $\mathcal{B}_0$; |
| $\tau^\alpha$ | Resolved shear stress on the $\alpha$th slip system; |
| $\sigma_{eq}$ | Equivalent stress; |
| $\gamma_\alpha$, $\dot{\gamma}_\alpha$ | Plastic slip, plastic slip rate; |
| $\varepsilon_{eq}$, $\dot{\varepsilon}_{eq}$ | Equivalent plastic strain, equivalent plastic strain rate. |

### 2.2. Kinematics

Consider a deformable body occupying configuration $\mathcal{B}_r$ in the reference state and configuration $\mathcal{B}$ in the current state. The total deformation gradient tensor $\mathbf{F}$ describes the linearized map between these two configurations.

The total deformation gradient tensor $\mathbf{F}$ can be multiplicatively split into an elastic $\mathbf{F}_e$ and plastic $\mathbf{F}_p$ contributions as follows:

$$\mathbf{F} = \mathbf{F}_e \cdot \mathbf{F}_p \,. \tag{1}$$

The multiplicative split introduces an intermediate configuration $\mathcal{B}_0$ distorted by the plastic deformation only. The elastic deformation, as well as rotations are included in $\mathbf{F}_e$. Fig. 1 sketches the three configurations with the related quantities that will be introduced in the following.

In the subsequent discussion, we will use the pull-back and push-forward operations, indicated by $\phi_e^*$ and $\phi_*^e$, respectively, along the elastic part of the deformation, i.e. from $\mathcal{B}$ to $\mathcal{B}_0$ and vice-versa.

We will make use of the metric tensor $\mathbf{g}$ of the current configuration. The pull-back of the current configuration metric to the intermediate configuration is the elastic Cauchy-Green tensor $\mathbf{C}_e = \phi_e^*\mathbf{g}$. Note that $\mathbf{C}_e = \mathbf{F}_e^T \cdot \mathbf{F}_e$. For the purpose of computation, it can be assumed $\mathbf{g} = \mathbf{I}$ (Cartesian coordinates), where $\mathbf{I}$ is the second-order identity tensor. However, in this section, we will consider the more general case of curvilinear coordinates to better highlight the origin of the proposed model equations. For a general derivation of hyperelastic–plastic models in the finite deformation setting, the reader is referred to e.g. (Simo et al., 1998; Belytschko et al., 2009).

We define the velocity gradient in the current configuration $\mathbf{L}$ and use the additive split into its elastic and plastic