COMPTES RENDUS
DE L'ACADÉMIE DES SCIENCES

Tome 340
fascicule 4–5

Avril–mai 2012
ISSN 1631-0721

MECANIQUE

Thematic issue / *Numéro thématique*
Recent Advances in Micromechanics of Materials
Guest editors / *Rédacteurs en chef invités :*
M. Bornert, R. Brenner, O. Castelnau,
P. Ponte Castañeda, P. Suquet

ACADÉMIE DES SCIENCES – PARIS

Recent Advances in Micromechanics of Materials

# Improved constitutive description of single crystal viscoplastic deformation by dislocation climb

Ricardo A. Lebensohn [a,*], R.A. Holt [b], A. Caro [a], A. Alankar [a], C.N. Tomé [a]

[a] *Materials Science and Technology Division, Los Alamos National Laboratory, MS G755, Los Alamos, NM 87545, USA*
[b] *Department of Mechanical and Materials Engineering, Queen's University at Kingston, K7L 3N6, Canada*

## ARTICLE INFO

## ABSTRACT

This article presents a continuum-level constitutive model of a single crystal deforming by dislocation climb, accounting for crystallography and dislocation/point-defect interactions. The proposed constitutive description represents an improvement over a previous recent model, which extended the rate-sensitivity approach for single crystal plasticity by dislocation glide to consider the deformation geometry of dislocation climb under the assumption of instantaneous restoration of equilibrium concentration of vacancies near climbing dislocations. The key element of the new model is a chemical stress parameter, which represents the additional driving force on climbing dislocations due the excess vacancy concentration. The original and new versions of the crystallographic model of climb are compared through a simple example of a strongly anisotropic single crystal that illustrates the differences in response due to the consideration or not of the chemical driving force for climb.

## 1. Introduction

At high homologous temperatures, and stresses above a certain threshold, materials deform in the thermal power-law creep regime, exhibiting rate-dependent plastic deformation carried by stress-assisted and thermally-activated dislocation motion [1]. This high-temperature plasticity regime can be further partitioned into a glide-controlled creep regime, under which the shear component of the applied stress acting along the glide direction on the glide plane is the one that drives dislocation movement. At higher temperatures, the interaction of dislocations with point defects permits the former to climb as well as glide. In this climb-controlled creep regime, the effect of the diagonal stress components must also be accounted for.

In a recent contribution [2], we considered the simultaneous activity of crystallographic climb and glide in a single crystal, and used the resulting continuum constitutive description to model the behavior of polycrystalline aggregates deforming in the climb-controlled creep regime. While single crystal plasticity models for glide-controlled deformation have been extensively used for more than 40 years, giving rise to an entire sub-field of research and applications within the broader field of computational plasticity, crystallographic models for the climb-controlled regime have been, strikingly, much less investigated and utilized. Besides our aforementioned contribution [2], previous works that made use of the geometry of climb at single crystal level to construct a polycrystal model are the formulations of Rougier et al. [3,4], and Tomé and Christodoulou [5] for the study of the irradiation-induced creep and growth of Zr-alloy polycrystals.

One strong assumption of our previous model [2] consisted in considering instantaneous restoration of equilibrium concentration of vacancies near climbing dislocations. This assumption allowed us to only consider the effect of the mechanical

---

* Corresponding author.
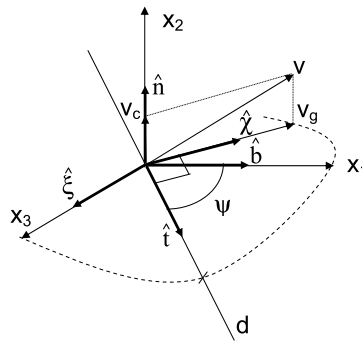  *E-mail address:* lebenso@lanl.gov (R.A. Lebensohn).

**Fig. 1.** Slip coordinate system and corresponding unit vectors $(\hat{\mathbf{b}}, \hat{\mathbf{n}}, \hat{\xi})$. Unit vectors of the dislocation coordinate system $(\hat{\mathbf{n}}, \hat{\mathbf{t}}, \hat{\chi})$. Dislocation line and dislocation velocity also shown.

component of the Peach–Koehler (PK) force acting on dislocations due to an external applied stress, disregarding the effect of the chemical PK component, related with the excess vacancy concentration generated by emission or absorption of the latter by climbing dislocations. In this contribution we present a new version of the crystallographic model for climb that incorporates a chemical stress parameter, which represents the additional driving force related to the non-equilibrium concentration of point defects in the crystal. The original and new versions of the climb model are compared through a simple example of a strongly anisotropic single crystal that illustrates the differences in response due to the consideration or not of this chemical driving force for climb.

## 2. Climb deformation geometry

The geometry of dislocation motion under stress can be described most simply in terms of a single dislocation of arbitrary orientation [6]. Let us consider the coordinate system $(x_1, x_2, x_3)$ shown in Fig. 1. The normal to the slip plane is specified by the unit vector $\hat{\mathbf{n}}$ along direction $x_2$. Dislocation motion produces a displacement $\mathbf{b}$ (Burgers vector) of the upper half of crystal in the direction of the unit vector $\hat{\mathbf{b}}$ along $x_1$. This slip coordinate system is completed by the unit vector $\hat{\xi} = \hat{\mathbf{b}} \times \hat{\mathbf{n}}$ along direction $x_3$. A general dislocation motion (i.e. by climb and glide) occurs in the direction of the velocity vector $\mathbf{v}$, which is normal to the dislocation line and has two components: the glide velocity, $v_g$, which lies in the slip plane, and the climb velocity, $v_c$, which is parallel to $\hat{\mathbf{n}}$. Another reference frame, the dislocation coordinate system, can be defined based on $\hat{\mathbf{t}}$, the tangent to the dislocation line, $\hat{\mathbf{n}}$, and $\hat{\chi}$, a unit vector parallel to $v_g$. Both the glide and climb velocity components arise in response to the corresponding component of the PK force on the dislocation. The Peach–Koehler force [7], a virtual force per unit length acting on a dislocation is defined as [8]:

$$\mathbf{f} = (\boldsymbol{\sigma} \cdot \mathbf{b}) \times \hat{\mathbf{t}} \tag{1}$$

from which we can define a glide component $f_g = \mathbf{f} \cdot \hat{\chi}$, and a climb component $f_c = \mathbf{f} \cdot \hat{\mathbf{n}}$ such that:

$$f_g = \left[(\boldsymbol{\sigma} \cdot \mathbf{b}) \times \hat{\mathbf{t}}\right] \cdot \hat{\chi} = (\boldsymbol{\sigma} \cdot \mathbf{b}) \cdot (\hat{\mathbf{t}} \times \hat{\chi}) = |\mathbf{b}|\boldsymbol{\sigma}' : (\hat{\mathbf{b}} \otimes \hat{\mathbf{n}}) \tag{2}$$

$$f_c = \left[(\boldsymbol{\sigma} \cdot \mathbf{b}) \times \hat{\mathbf{t}}\right] \cdot \hat{\mathbf{n}} = (\boldsymbol{\sigma} \cdot \mathbf{b}) \cdot (\hat{\mathbf{t}} \times \hat{\mathbf{n}}) = -|\mathbf{b}|\boldsymbol{\sigma} : (\hat{\mathbf{b}} \otimes \hat{\chi}) \tag{3}$$

Last equality in Eq. (2), involving only the deviatoric component of the stress $\boldsymbol{\sigma}'$, follows from the normality between $\hat{\mathbf{b}}$ and $\hat{\mathbf{n}}$. The climb force, on the other hand, depends on the full Cauchy stress, $\boldsymbol{\sigma}$. However, thermodynamic considerations by Weertman (see [9] for details), led to a modification of Eq. (3), involving a distinction between a mechanical component produced by an applied stresses, and a chemical component due to non-equilibrium concentration of point defects (vacancies, in the case of thermal creep), such that [9]:

$$\mathbf{f} = (\boldsymbol{\sigma}' \cdot \mathbf{b}) \times \hat{\mathbf{t}} + \left[ -\frac{k_B T}{\alpha |\mathbf{b}|^3} \log(x_v / x_v^{0,PT}) \right] \mathbf{b} \times \hat{\mathbf{t}} \tag{4}$$

where $\alpha |\mathbf{b}|^3$ is the volume change due to the formation of a vacancy and the first and second terms on the right are the mechanical and chemical components of the PK force, respectively. In the expression for the chemical force, $x_v$ is the actual concentration of vacancies, $x_v^{0,PT}$ is the equilibrium concentration of vacancies at the crystal's hydrostatic pressure $P$ and temperature $T$, and $k_B$ is Boltzmann's constant. Therefore, while the expression of the glide component remains the same, the climb component should be re-written as:

$$f_c = -|\mathbf{b}|\boldsymbol{\sigma}' : (\hat{\mathbf{b}} \otimes \hat{\chi}) - |\mathbf{b}| \left[ -\frac{k_B T}{\alpha |\mathbf{b}|^3} \log(x_v / x_v^{0,PT}) \right] (\hat{\mathbf{b}} \otimes \hat{\chi}) \tag{5}$$

If the vacancy concentration in the crystal is everywhere equal to the equilibrium concentration at pressure $P$ and temperature $T$, the chemical force becomes zero. This condition is possible if the sources and sinks for vacancies (dislocations and

surfaces) are such that vacancies are instantaneously produced or annihilated by these sources and sinks to maintain the required equilibrium concentration.

The dyadic product in Eq. (2) is the classic glide tensor, which can be decomposed into symmetric and antisymmetric parts:

$$\mathbf{g} = \hat{\mathbf{b}} \otimes \hat{\mathbf{n}} = \mathbf{m} + \mathbf{q} = \frac{1}{2}(\hat{\mathbf{b}} \otimes \hat{\mathbf{n}} + \hat{\mathbf{n}} \otimes \hat{\mathbf{b}}) + \frac{1}{2}(\hat{\mathbf{b}} \otimes \hat{\mathbf{n}} - \hat{\mathbf{n}} \otimes \hat{\mathbf{b}}) \tag{6}$$

where $m_{ij}$ is the symmetric Schmid tensor and $q_{ij}$ is the corresponding antisymmetric (plastic rotation) tensor (note that since $\hat{\mathbf{b}} \perp \hat{\mathbf{n}}$, $g_{ij}$ and $m_{ij}$ are traceless). The product $\boldsymbol{\sigma}' : (\hat{\mathbf{b}} \otimes \hat{\mathbf{n}}) = \mathbf{m} : \boldsymbol{\sigma}'$ is the resolved shear stress (i.e. the $\sigma'_{12}$ component of the external stress tensor expressed in slip-system coordinates), which, according to the Schmid law, has to reach a threshold value for slip activation. Eq. (2) thus provides a physical interpretation of the phenomenological Schmid law, i.e. slip is activated when a critical value of the force acting on dislocations is reached to overcome the slip resistance and start dislocation motion. The Schmid law has been modified to account for rate effects and multislip, giving raise to the widely used rate-sensitivity constitutive equation for single crystal material points deforming plastically by glide [10], i.e.

$$\dot{\varepsilon}_{ij}^{\prime g} = \sum_{s=1}^{N_s} m_{ij}^s \dot{\gamma}^s = \dot{\gamma}_o \sum_{s=1}^{N_s} m_{ij}^s \left( \frac{|\mathbf{m}^s : \boldsymbol{\sigma}'|}{\tau_{o,g}^s} \right)^{n_g} \operatorname{sgn}(\mathbf{m}^s : \boldsymbol{\sigma}') \tag{7}$$

where $\dot{\boldsymbol{\varepsilon}}'^g$ is the (traceless) plastic strain rate tensor induced by glide. In the expression above the sum runs over all $N_s$ active slip systems; $\mathbf{m}^s$ and $\tau_{o,g}^s$ are, respectively, the Schmid tensor and the threshold resolved shear stress associated with glide in system (s); $\dot{\gamma}^s$ is the shear rate on slip system (s); $\dot{\gamma}_o$ is a normalization factor and $n_g$ is the stress exponent (inverse of the rate-sensitivity) associated with glide.

By analogy with the above constitutive description of a single crystal deforming plastically by glide, the dyadic product appearing in Eq. (5) can be defined as a climb tensor [2,6], i.e.

$$\mathbf{c} = \hat{\mathbf{b}} \otimes \hat{\boldsymbol{\chi}} = \mathbf{k} + \mathbf{r} = \frac{1}{2}(\hat{\mathbf{b}} \otimes \hat{\boldsymbol{\chi}} + \hat{\boldsymbol{\chi}} \otimes \hat{\boldsymbol{b}}) + \frac{1}{2}(\hat{\mathbf{b}} \otimes \hat{\boldsymbol{\chi}} - \hat{\boldsymbol{\chi}} \otimes \hat{\boldsymbol{b}}) \tag{8}$$

where $k_{ij}$ and $r_{ij}$ are, respectively, the symmetric and antisymmetric parts of the climb tensor. The climb tensor resolves the stress into a climb component in the same way the glide tensor does for the glide component. However, there are some important differences between the two tensors. While $g_{ij}$ is formed from two unit vectors based on the crystallography of the slip process independently of the dislocation line orientation, $c_{ij}$ depends on the orientation (character) of the dislocation. This dependence can be expressed in terms of $\psi$, i.e. the angle between $\hat{\mathbf{t}}$ and $\hat{\mathbf{b}}$. This parameter accounts for the relative edge-screw character of the average dislocation density. In addition, it is evident that the climb tensor is in general non-traceless. Hence, the symmetric climb tensor can be further decomposed into a deviatoric and a hydrostatic component, i.e.

$$\mathbf{k} = \mathbf{k}^d + \mathbf{k}^h \tag{9}$$

The deviatoric, hydrostatic and antisymmetric components of the climb tensor expressed in slip-system coordinates are [6]:

$$\mathbf{k}^d = \frac{1}{6} \begin{bmatrix} 4\sin\psi & 0 & 3\cos\psi \\ 0 & -2\sin\psi & 0 \\ 3\cos\psi & 0 & -2\sin\psi \end{bmatrix} \tag{10}$$

$$\mathbf{k}^h = \frac{1}{3} \begin{bmatrix} \sin\psi & 0 & 0 \\ 0 & \sin\psi & 0 \\ 0 & 0 & \sin\psi \end{bmatrix} \tag{11}$$

$$\mathbf{r} = \frac{1}{2} \begin{bmatrix} 0 & 0 & \cos\psi \\ 0 & 0 & 0 \\ -\cos\psi & 0 & 0 \end{bmatrix} \tag{12}$$

Carrying on the analogy with the constitutive description of glide, we proposed [2] to treat climb as being activated when the climb force acting on dislocations reaches a critical value. In the case of equilibrium concentration of vacancies, a scalar climb rate on system (s) can be defined as:

$$\dot{\beta}^s = \dot{\gamma}_o \left( \frac{|\mathbf{k}^{d,s} : \boldsymbol{\sigma}'|}{\tau_{o,c}^s} \right)^{n_c} \operatorname{sgn}(\mathbf{k}^{d,s} : \boldsymbol{\sigma}') \tag{13}$$

where $n_c$ and $\tau_{o,c}^s$ are, respectively, the stress exponent and a scalar threshold stress associated with climb. This definition leads to the following total strain rate of a single crystal deforming by climb (cf. Eq. (7)):

$$\dot{\varepsilon}_{ij}^{\prime c} = \sum_{s=1}^{N_s} k_{ij}^{d,s} \dot{\beta}^s = \dot{\gamma}_o \sum_{s=1}^{N_s} k_{ij}^{d,s} \left( \frac{|\mathbf{k}^{d,s} : \boldsymbol{\sigma}'|}{\tau_{o,c}^s} \right)^{n_c} \mathrm{sgn}(\mathbf{k}^{d,s} : \boldsymbol{\sigma}') \tag{14}$$

Like their glide counterparts ($n_g$ and $\tau_{o,g}^s$), parameters $n_c$ and $\tau_{o,c}^s$ depend on temperature, strain rate and microstructure. Eq. (14) allows one, e.g., to obtain the 5 independent components of the deviatoric strain rate of the crystal for an applied deviatoric stress, or to solve a $5 \times 5$ system of non-linear equations to obtain $\boldsymbol{\sigma}'$ for a strain rate imposed to the crystal.

## 3. Accounting for dislocation/point defect interaction

In order to account for the chemical component of the PK force acting on climbing dislocations, we propose to modify Eq. (14) in the following way:

$$\dot{\varepsilon}_{ij}^{c} = \dot{\gamma}_o \sum_{s=1}^{N_s} k_{ij}^s \left( \frac{|\mathbf{k}^{d,s} : \boldsymbol{\sigma} + \tau^{ch}|}{\tau_{o,c}^s} \right)^{n_c} \mathrm{sgn}(\mathbf{k}^{d,s} : \boldsymbol{\sigma} + \tau^{ch}) \tag{15a}$$

$$\dot{\varepsilon}_{kk}^{c} = 0 \tag{15b}$$

where the chemical stress parameter $\tau^{ch}$ is scalar quantity that represents the dragging or boosting effect of the positive or negative excess concentration of vacancies, with respect to the equilibrium concentration at the crystal's temperature and pressure in the absence of external applied stresses. This new constitutive parameter $\tau^{ch}$ is evidently related with the second term on the right of Eq. (5) that gives the climb component of the PK force acting on dislocations in crystals with non-equilibrium concentration of point defects. The introduction of this parameter, adding (or subtracting) from the resolved climb stress is inspired in the constitutive treatment of kinematic hardening (e.g. see in [11] the generalization to crystal plasticity of the classic isotropic kinematic hardening formulation [12]), in which the kinematic hardening parameter represents the effect of back-stresses produced by dislocation structures generated during previously accumulated plastic deformation by slip. However, while kinematic hardening parameters should be, in general, identified for each slip system, the chemical stress parameter is unique for the entire crystal (or a single-crystal material point), and its value is not imposed, but it follows from the resolution of the system of non-linear equations given by Eq. (15) and the applied boundary conditions. Note that the introduction of $\tau^{ch}$ as a new unknown requires adding the incompressibility condition (Eq. (15b)) explicitly, in order to solve a $6 \times 6$ system, instead of a $5 \times 5$ one (cf. Eq. (14)). Next section illustrates the use of Eq. (15) in the case of a strongly anisotropic single crystal deforming only by climb.

## 4. Application

The original [2] and the present new version of the crystallographic model of climb are hereby compared through a simple example of a strongly anisotropic single crystal that illustrates the differences in response due to the consideration or not of the chemical driving force for climb. Fig. 2(a) shows the initial geometry of the problem, with the two available edge dislocation systems $S_1$ and $S_2$, and an applied Cauchy stress, of the form:

$$\boldsymbol{\sigma}^{app} = \begin{bmatrix} \sigma_{11}^{app} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{16}$$

resulting in deviatoric stress components $\sigma_{11}^{\prime app} = 2/3\sigma_{11}^{app}$ and $\sigma_{22}^{\prime app} = \sigma_{33}^{\prime app} = -1/3\sigma_{11}^{app}$. Note that the mechanical driving force acting on $S_1$ dislocations ($\sigma_{11}^{\prime app}$) is twice the one on $S_2$ dislocations ($\sigma_{22}^{\prime app}$) and that deformation along $x_3$ cannot be accommodated by climb of either dislocation types. In order to simplify the analysis, we adopt the following values for the model parameters and applied stress: $\tau_{o,c}^s = 1$; $n_c = 1$; $\dot{\gamma}_o = 1$ and $\sigma_{11}^{app} = 1$. With these numerical values, the climb tensors and the corresponding stress projections on them are:

$$\mathbf{k}^{s_1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}; \quad \mathbf{k}^{d,s_1} = \begin{bmatrix} 2/3 & 0 & 0 \\ 0 & -1/3 & 0 \\ 0 & 0 & -1/3 \end{bmatrix} \tag{17a}$$

$$\mathbf{k}^{s_2} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}; \quad \mathbf{k}^{d,s_2} = \begin{bmatrix} -1/3 & 0 & 0 \\ 0 & 2/3 & 0 \\ 0 & 0 & -1/3 \end{bmatrix} \tag{17b}$$

$$\mathbf{k}^{d,s_1} : \boldsymbol{\sigma}^{app} = \frac{2}{3}; \quad \mathbf{k}^{d,s_2} : \boldsymbol{\sigma}^{app} = -\frac{1}{3} \tag{17c}$$

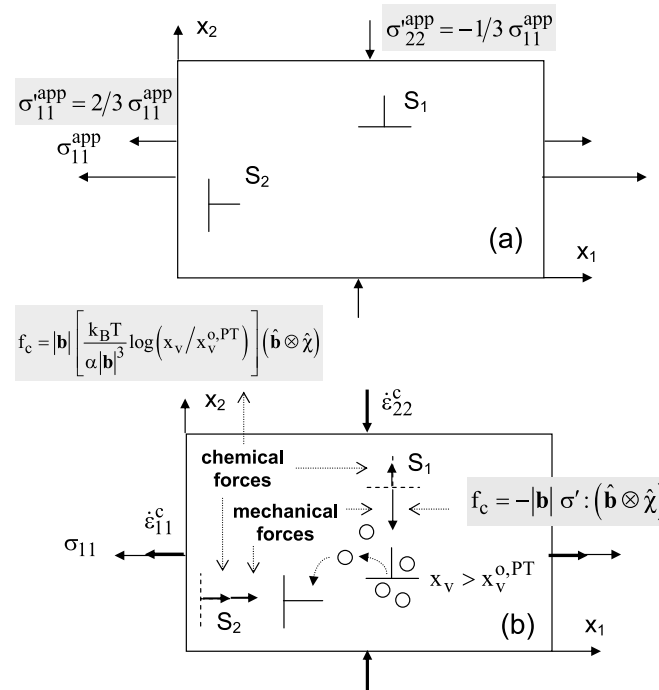Replacing these values in Eq. (15a) we obtain:

**Fig. 2.** Strongly anisotropic single crystal deforming by dislocation climb. (a) Initial configuration, showing the applied stress, and the two available dislocation systems. Mechanical driving force acting on $S_1$ dislocations ($\sigma_{11}'^{\mathrm{app}}$) is double than the one on $S_2$ dislocations ($\sigma_{22}'^{\mathrm{app}}$). Deformation along $x_3$ cannot be accommodated by climb of either dislocation types. (b) Schematic representation of dislocation climb, with indication of the mechanical and chemical components of the PK force acting on the climbing dislocations. The concentration of vacancies in the crystal is above the equilibrium concentration. The resulting $\dot{\varepsilon}_{11}^c$ and $\dot{\varepsilon}_{22}^c$ strain rate components are respectively equal in magnitude and of opposite sign, while $\dot{\varepsilon}_{33}^c$ is zero.

$$\dot{\boldsymbol{\varepsilon}}^c = \begin{bmatrix} 2/3 + \tau^{\mathrm{ch}} & 0 & 0 \\ 0 & -1/3 + \tau^{\mathrm{ch}} & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{18}$$

which, combined with the incompressibility condition (15b) gives:

$$\dot{\varepsilon}_{11}^c = 1/2; \qquad \dot{\varepsilon}_{22}^c = -1/2; \qquad \dot{\varepsilon}_{33}^c = 0 \quad \text{and} \quad \tau^{\mathrm{ch}} = -1/6 \tag{19}$$

Fig. 2(b) shows a schematic representation of the climb process, with indication of the mechanical and chemical components of the PK force acting on both types of dislocations. Note that, from Eq. (5), the mechanical PK components have opposite sign with respect to the projections of the applied stress on the climb tensors (Eq. (17c)). Evidently, the fact that the mechanical driving force on $S_1$ dislocations (which need to emit vacancies to climb, extending the extra lattice plane downwards and thus the crystal in $x_1$ direction) is twice the one on $S_2$ dislocations (which absorb vacancies, moving the extra plane to the right and contracting the crystal in $x_2$ direction) gives an overall concentration of vacancies in the crystal above the equilibrium concentration ($x_v > x_v^{o,PT}$). This determines a positive chemical PK component, which opposes (i.e. drags) $S_1$ dislocations, and adds to the mechanical component acting on $S_2$ dislocations, respectively. The incompressibility condition and the fact that there are no dislocations able to accommodate strain in the $x_3$ direction results in strain rate components $\dot{\varepsilon}_{11}^c$ and $\dot{\varepsilon}_{22}^c$ of equal magnitude and opposite sign, and $\dot{\varepsilon}_{33}^c = 0$.

Note also that the absolute value of the chemical stress parameter $\tau^{\mathrm{ch}}$, besides depending on the relative orientation of the available dislocation systems with respect to the applied stress, also depends on the magnitude of this stress. In the example, if the applied stress increases, the absolute value of $\tau^{\mathrm{ch}}$ will also increase, reflecting an increase of $x_v$ and a stronger bias of towards vacancy emission with respect to absorption by climbing dislocations.

It is interesting to compare the above response, predicted by means of the new constitutive framework, with the one that is obtained with the previous version of the climb model [2], i.e. using Eq. (14), for the same boundary conditions and assuming the same numerical values for the model parameters. Plugging the numbers given by (17) in Eq. (14) gives:

$$\dot{\varepsilon}_{11}^c = 5/9; \qquad \dot{\varepsilon}_{22}^c = -4/9; \qquad \dot{\varepsilon}_{33}^c = -1/9 \tag{20}$$

Evidently, neglecting the effect of the non-equilibrium concentration of vacancies determines a faster extension ($\dot{\varepsilon}_{11}^c = 5/9 > 1/2$) in the $x_1$ direction, meaning that the climb of $S_1$ dislocations, responsible for this extension, is facilitated by neglecting the dragging effect of the excess vacancy concentration, and a slower contraction ($\dot{\varepsilon}_{22}^c = -4/9 > -1/2$) in the $x_2$ direction, i.e. the climb of $S_2$ dislocations is only driven by the external stress, without the chemical component boost. Interestingly, despite that none of the dislocation types can accommodate strain along $x_3$, in this case the resulting $\dot{\varepsilon}_{33}^c$ does not vanish. This negative strain rate component along $x_3$ can be explained as follows. Since the original climb model

was constructed under the assumption of instantaneous restoration of the equilibrium concentration of vacancies, the actual overall excess of vacancies made evident by the previous analysis should go somewhere, i.e. to dislocations or surfaces. For this configuration, the model results imply that part of these excess vacancies are absorbed at a surface with normal along direction $x_3$, determining a contraction of the crystal in that direction.

## 5. Summary and perspectives

We have presented and assessed a new version of a constitutive model for single crystals deforming by thermal creep, with explicit account of the geometry of climb. The proposed constitutive framework is built upon our previous crystallographic climb model [2], including an improved description of an important underlying physical mechanism, the dislocation/point-defect interaction. The newly introduced chemical stress parameter accounts for the effect of non-equilibrium concentrations of vacancies, arising from the fact that, due to the intrinsic single crystal anisotropy, the climb driving forces of mechanical origin rarely determine that the vacancies emitted at certain rates by dislocations climbing in one direction (e.g. in the case of edge dislocations, extending the extra lattice plane) can be absorbed at the same rate by dislocations climbing in the other direction (e.g. removing atoms from the extra plane).

While the model equations and examples were given here for the case of thermal creep, in which only vacancies (and not interstitials, due of their very low concentration) are relevant to promote dislocation climb, the formulation can be extended to irradiation creep. In this case, vacancies and interstitials are continuously created in pairs, leading to a supersaturation of point defects in the irradiated crystal, which only allows for climbing of dislocations by absorption (not emission) of either type of defect, depending on the sign of the driving force. Since vacancies and interstitials interact with dislocations differently, the extension of the proposed constitutive description to irradiation creep should involve some kind of polarity, i.e. the threshold stress for climb should be different, depending on the sign of the resolved stress for climb plus the chemical stress. This difference will reflect the fact that the type of point defects to be absorbed depends on the direction of climb. In such case, Eq. (15) may be modified as follows:

$$
\left| \begin{array}{l}
\dot{\varepsilon}_{ij}^{c} = \dot{\gamma}_0 \sum_{s=1}^{N_s} k_{ij}^{s} \left( \frac{|\mathbf{k}^{d,s} : \boldsymbol{\sigma}' + \tau^{ch}|}{\tau_{o,c}^{s}(\mathrm{sgn}(\mathbf{k}^{d,s} : \boldsymbol{\sigma}' + \tau^{ch}))} \right)^{n_c} \mathrm{sgn}(\mathbf{k}^{d,s} : \boldsymbol{\sigma}' + \tau^{ch}) \\
\dot{\varepsilon}_{kk}^{c} = 0
\end{array} \right.
\tag{21}
$$

and two (i.e. $\tau_{o,c}^{s+}$ and $\tau_{o,c}^{s-}$) instead of one threshold stresses should be identified, one for climb by absorption of vacancies and another of interstitials.

In the case presented here, we restricted the analysis to pure climb. However, in the more general case in which creep is controlled by climb but most of the dislocation motion is by glide, both glide (Eq. (7)) and climb (Eq. (14)) contributions should be considered and, most importantly, the complicated coupling between climb and glide (e.g. when a gliding dislocation stops at an obstacle, a small amount of climb may allow it to overcome the obstacle and continue gliding, providing a significant amount of strain until it reaches the next obstacle, and so on) should be accounted for. This will require the addition of sophisticated hardening laws, involving the mutual influence of the glide and climb strains on the evolution of the glide and climb threshold stresses.

The determination of the threshold stress for climb can be either done by inverse analysis of experimental data, or using lower length-scale models to obtain the stress needed to move dislocations by climb in the presence of certain concentration of point defects. This can be done semi-analytically by means of rate-theory (e.g. [13]), or by numerical schemes like dislocation dynamics (e.g. [14]), or molecular dynamics/kinetic Monte Carlo techniques (e.g. [15]).

Finally, it should be mentioned that the proposed single crystal model can be readily implemented as part of a polycrystal formulation, as done in [2] utilizing self-consistent homogenization, or within the context of full-field models, e.g. based on crystal-plasticity finite elements or spectral methods. Efforts in this direction are presently under way [15].

## Acknowledgements

## References

[1] H.J. Frost, M.F. Ashby, Deformation-Mechanism Maps, Pergamon Press, Oxford, 1982.
[2] R.A. Lebensohn, C.S. Hartley, C.N. Tomé, O. Castelnau, Modelling the mechanical response of polycrystals deforming by climb and glide, Phil. Mag. 90 (2010) 567–583.
[3] Y. Rougier, T. Bretheau, A. Zaoui, A new approach to determine the zircaloy constitutive behavior under irradiation, in: K.F. Kussmaul (Ed.), Proceedings of SMiRT-12, Stuttgart, 1993.
[4] Y. Rougier, Etude du comportement sous irradiation: modélisation micromécanique de l'elastoviscoplasticite, PhD thesis, Ecole Polytechnique, Palaiseau, France, 1994.
[5] C.N. Tomé, N. Christodoulou, Analysis of accelerated irradiation growth in Zr–2.5% Nb pressure tubes, Phil. Mag. 80 (2000) 1407–1424.

[6] C.S. Hartley, A method for linking thermally activated dislocation mechanisms of yielding with continuum plasticity theory, Phil. Mag. 83 (2003) 3783–3808.

[7] M. Peach, J.S. Koehler, The forces exerted on dislocations and the stress fields produced by them, Phys. Rev. 80 (1950) 436–439.

[8] J.P. Hirth, J. Lothe, Theory of Dislocations, McGraw–Hill, New York, 1968.

[9] J. Weertman, The Peach–Koehler equation for the force on a dislocation modified for hydrostatic pressure, Phil. Mag. 11 (1965) 1217–1223.

[10] R.J. Asaro, A. Neddleman, Texture development and strain hardening in rate-dependent polycrystals, Acta Metall. 33 (1985) 923–953.

[11] G. Cailletaud, A micromechanical approach to inelastic behaviour of metals, Int. J. Plasticity 8 (1992) 55–73.

[12] J.L. Chaboche, Constitutive equations for cyclic plasticity and cyclic viscoplasticity, Int. J. Plasticity 5 (1989) 247–302.

[13] R. Bullough, M.W. Finnis, M.H. Wood, A theory of irradiated and thermal creep by dislocation climb, J. Nucl. Mater. 103 (1982) 1263–1268.

[14] D. Mordehai, E. Clouet, M. Fivel, M. Verdier, Introducing dislocation climb by bulk diffusion in discrete dislocation dynamics, Phil. Mag. 88 (2008) 899–925.

[15] A. Alankar, et al., in preparation.