

A numerical procedure enabling accurate descriptions of strain rate-sensitive flow of polycrystals within crystal visco-plasticity theory

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Highlights

- A method enabling crystal visco-plasticity to consider realistic rate-sensitivity exponents is developed.
- The method separates constant structure (the exponent) from evolving structure (the activation stress) rate-sensitivity.
- The method within VPSC is applied to simulate strain rate-sensitive deformation of Cu from 10^{-4} /s to 10^4 /s.
- The method does not increase the computation time involved in polycrystal simulations.

Abstract

The plastic deformation of polycrystalline metals is carried by the motion of dislocations on specific crystallographic glide planes. According to the thermodynamics theory of slip, in the regime of strain rates, roughly from 10^{-5} /s to 10^5 /s, dislocation motion is thermally activated. Dislocations must overcome barriers in order to move, and this concept defines critical activation stresses τ_c^s on a slip system s that evolve as a function of strain rate and temperature. The fundamental flow rule in crystal visco-plasticity theory that involves τ_c^s in order to activate slip has a power-law form: $\dot{\gamma}^s = \dot{\gamma}_0 \left(\frac{|\tau^s|}{\tau_c^s} \right)^n \text{sign}(\tau^s)$. This form is desirable because it provides uniqueness of solution for the active slip systems that accommodate an imposed strain rate; however, it also introduces a strain rate dependence, which in order to represent the actual behavior of polycrystalline materials deforming in relevant conditions of temperature and strain-rate usually needs to be described by a high value of the exponent n . However, since until now the highest value of n was limited by numerical tractability, the use of the power-law flow rule frequently introduced an artificially high rate-sensitivity. All prior efforts to correct this extraneous rate sensitivity have only lessened its effect and unfortunately also at the expense of substantial increases in computation time. To this day, a solution for the power-law exponent reflecting true material behavior is still sought. This article provides a novel method enabling the use of realistic material strain rate-sensitivity exponents to be used within the crystal visco-plasticity theory without increasing computation time involved

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in polycrystal simulations. Calculations are performed for polycrystalline pure Cu and excellent agreement with experimental measurement is demonstrated.

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1. Introduction

Much of the physics of plastic deformation and the role of dislocation motion in it were known before the development of crystal plasticity based models. Dislocation glide marks over polished and deformed surfaces of metallic samples were reported before 1900 [1,2]. It was then concluded that dislocation glide on specific crystallographic planes and directions lying on those planes and their glide imparts the needed shear to deform the crystal. It was also observed that not all crystallographically equivalent planes and directions in a crystal were active during plastic deformation.

Later, the theory of the thermodynamics of slip was developed. It builds on the idea that dislocation motion is thermally activated in the strain rate ranging roughly from 10^{-5} /s to 10^5 /s [3,4]. The critical stress τ_c^s to move dislocations on an individual system is generally comprised of two components. The first is an intrinsic athermal stress, representing lattice friction and hence thought not to depend on strain rate within the aforementioned thermally activated regime. The second is a dislocation-interaction term, which is controlled by overcoming obstacles on the glide plane, such as other intersecting dislocations, and would generally depend on both strain rate and temperature. τ_c^s depends on chemical composition and evolves as the microstructure within the grain evolves, which includes for instance, dislocation storage, twinning, and substructure development [5–9]. This rate-sensitive dislocation motion occurs within every plastically deforming crystal in the polycrystalline aggregate and causes the macroscopic flow stress–strain response of the polycrystal to depend strongly on the applied stress, strain rate, and temperature of deformation [10,11]. A current overarching aim of materials modeling is to relate the rate-sensitive motion of dislocations to the deformation of a crystal or set of crystals when strained at a particular temperature and strain rate.

An essential and critical part of this modeling effort is the adoption of a sound criterion (or criteria) for activating crystallographic slip. However, the fact that crystal deformation generally involves slip on more than one slip system makes this a challenging task. Most pure metals with a face centered cubic crystal structure (e.g., Cu, Ni, Al) deform on one slip family $\{111\}$ $(1\bar{1}0)$, which contains twelve independently oriented slip systems [12–14]. Metals, such as steel and most of refractory metals, with a body-centered cubic crystal structure, have two or three families, making up 24 or 48 slip systems [15–19]. Metals with a lower symmetry crystal structure, like hexagonal close packed Mg, Zr, Be, or Ti metals or orthorhombic U, possess an even larger suite of slip families and systems [20–25]. When plastically deformed, a crystal accommodates strain using a small subset of these systems. Which systems are activated, how many, and the distribution of shear among them are collectively referred to as slip activity.

Predicting slip activity is fundamental to be able to predict the reorientations of the crystals and material flow stress with strain. The theory of crystal plasticity can predict slip activity and relate it to the geometry of crystal deformation; however, it still requires a separate and basic criterion for activating an individual slip system. All polycrystal plasticity based constitutive models, ranging from mean-field models, such as the upper bound Taylor model [26], lower bound Sachs model [27], and the various self-consistent schemes, such as visco-plastic self-consistent (VPSC) [28,29], to the full-field crystal plasticity finite element (CPFE) [30–33] and Fast Fourier Transform-based (CP-FFT) [34] techniques, require a criterion for activating a slip system in order to predict slip activity. It is desirable that this criterion captures the rate sensitive motion of dislocations.

The strain rate and temperature sensitivity of the plastic deformation response of metals can in general be represented through the flow stress. The strain-rate sensitivity has been shown to be well represented by several constitutive models that are based on thermal activation kinetics developed by Kocks et al. [13]. One primary example is the mechanical threshold stress (MTS) model, which is due to the work of Follansbee and Kocks [35] and has been used in several applications involving dynamic deformation of materials [36, 37], including an extension to crystal plasticity by assigning a MTS to each slip system [38]. In this

model, the internal state variable, i.e. the MTS, is the deformation resistance at 0 °K, and the flow rule is a combination of log and power law. Other examples treat the rate sensitivity of the material in a completely general fashion and use other forms for the flow rule, i.e. not necessarily an exponential law or a power law, and several internal parameters therein are a function of the strain-rate and temperature (e.g. [39–42]). This more general and flexible dependence comes at the expense of a laborious tabulation of model parameters from experiments. The new algorithm presented in this paper avoids such time-consuming tabulation, provided the critical stress dependence with strain-rate can be described by a single stress exponent, which is often a reasonable assumption.

The criterion adopted by many visco-plastic crystal deformation models is the flow rule that relates the rate of slip on slip system s to the stress resolved on the slip system plane and direction [43], i.e.,

$$\dot{\gamma}^s = \dot{\gamma}_0 \left(\frac{|\boldsymbol{\sigma}' \cdot \mathbf{b}^s \otimes \mathbf{n}^s|}{\tau_c^s} \right)^n \text{sign}(\boldsymbol{\sigma}' \cdot \mathbf{b}^s \otimes \mathbf{n}^s) \quad (1)$$

where \mathbf{n}^s and \mathbf{b}^s are the slip plane normal and direction of slip system s , $\dot{\gamma}^s$ is the slip rate on s , $\boldsymbol{\sigma}'$ is the deviatoric Cauchy stress tensor, n is the power-law exponent, and τ_c^s is the slip resistance for a given microstructural state. We denote the dot product by “ \cdot ” and the tensor product by “ \otimes ”. The exponent n is the slip system-level equivalent of the inverse of the strain rate sensitivity parameter m , which represents the dependence of the activation stress on strain rate for fixed τ_c^s , or equivalently, at fixed microstructure. The strain-rate sensitivity of material response m is $1/n$ with n defined as the slope of the ln–ln stress–strain rate curve [35,44]:

$$n = \left. \frac{\partial \ln \dot{\epsilon}}{\partial \ln \sigma} \right|_{\epsilon} \quad (2)$$

The value of n depends on material and is established experimentally from flow stresses at different strain rates but the same microstructural state (e.g., dislocation density storage). For Cu, for instance, the strain rate sensitivity is approximately $m = 0.0025$, which is a relatively low value yielding n of 400 [35]. Similarly high n values also apply to other metals such as brass, aluminum alloys, many steels etc. [44]. While for cubic metals the same n value can be assigned for all slip systems [43,45], usually n value varies per slip mode for low symmetry metals, which deform by multiple slip modes [46]. For Mg, for instance, it is widely accepted that basal slip exhibits a very low strain rate sensitivity of approximately 10^{-6} while prismatic and pyramidal slip have much higher values 0.0235 and 0.00742, respectively [47–49]. Low-symmetry metals also deform by deformation twinning, whose propagation is usually considered rate insensitive compared to slip [50]. Note that this rate sensitivity embedded in the rate sensitivity exponent is in addition to the rate-sensitive evolution of τ_c^s , as dictated by the thermodynamics of slip [4,35].

The power-law form is highly desired as it provides uniqueness in solution that other criteria do not. However, due to numerical limitations, the exponent n used for example in VPSC or CP-FFT is typically 20. The significantly higher n values needed to accurately reflect the actual material strain rate sensitivity at constant microstructure τ_c^s is difficult to obtain while preserving reasonable computational efficiency of the codes. Use of low values of n introduces an inaccurate coupling between the rate-sensitive macroscopic response and rate-sensitive evolution of τ_c^s . This problem is widely recognized, and as we describe below, over the years, there have been attempts to resolve it but none of them have been able to achieve values of n representative of actual materials (>100) [38,44,51].

In this article, we introduce a novel and computationally efficient numerical procedure to allow for a wide range of values for the exponent reflecting material strain rate-sensitivity m , including extremely low values of 0.001 or as low as necessary to accurately describe strain rate sensitive flow of polycrystals. Hence, the procedure enables the use of realistic strain rate sensitivity exponents, which are true visco-plastic properties for polycrystalline metals. The article provides a brief historical perspective, then develops the method, called the k -modification (k -mod) method, and ends with demonstration of its utility in a multiscale crystal plasticity constitutive model for the strain rate-sensitive deformation behavior of polycrystalline Cu, which exhibits a relatively low strain rate-sensitivity and hence large value of n . Excellent agreement with experimental measurement is shown. This development marks the first time a polycrystal visco-plasticity model implementation able to represent thermally activated dislocation motion across

nm–mm length scales in quantitative agreement with a wide range of experimental conditions, without immeasurable, superfluous strain rate effects entering numerically via the slip activation criterion.

2. Background

2.1. Rate-independent onset of slip criterion

The first criterion developed for activating slip is perhaps still to date the most intuitive one, making the most physical sense. It is the rate-independent criterion. In 1923, it was postulated that the resolved shear stress has to reach a critical value τ_c^s in order for slip to become active on a particular plane in a particular direction [52]. The concept was later refined and became known as the Schmid law [53]. This criterion can be expressed as:

$$\dot{\gamma}^s = 0, \quad \text{if } |\tau^s| < \tau_c^s \tag{3a}$$

$$\dot{\gamma}^s \neq 0, \quad \text{if } |\tau^s| \geq \tau_c^s \quad \text{sign}(\dot{\gamma}^s) = \text{sign}(\tau^s) \tag{3b}$$

and represents the activation of slip on a slip system s . We introduce ‘ c ’ to reflect crystal quantities. The stress measure $\tau^s = \sigma'^c \cdot \mathbf{m}^{sc}$ is the resolved shear stress on slip system s and $\mathbf{m}^{sc} = \frac{1}{2}(\mathbf{b}^s \otimes \mathbf{n}^s + \mathbf{n}^s \otimes \mathbf{b}^s)$ is symmetric portion of the system’s Schmid tensor. The strain rate tensor for the single crystal, $\dot{\epsilon}_{vp}^c$, is related to all its active slip systems, via:

$$\dot{\epsilon}_{vp}^c = \sum_s \dot{\gamma}^s \mathbf{m}^{sc}, \tag{4}$$

where

$$\dot{\gamma}^s = \dot{\gamma}_0 \text{sign}(\tau^s), \tag{5}$$

where $\dot{\gamma}_0$ is usually arbitrarily selected as the scaling factor such that $\dot{\epsilon}_{vp}^c$ is similar in value to the macroscopic viscoplastic strain rate.

This criterion is rate independent since the formulation does not introduce a rate dependency separate from τ_c^s . Because of rate-independency, a constant and fixed τ_c^s would result in the same activation stresses for slip for all strain rates. This criterion still allows for the evolution of the critical threshold τ_c^s to depend on strain rate and temperature. The term “rate-independent” approach is disconnected from the fact that the rate sensitivity of dislocation motion can still be embodied in τ_c^s .

The challenge in using this criterion in crystal plasticity formulations lies in determining how many slip systems are active in the crystal. With it, multiple combinations of active slip systems can provide the same $\dot{\epsilon}_{vp}^c$. The most generic $\dot{\epsilon}_{vp}^c$ can be satisfied with five independent slip systems. The finding of a unique set of five independent slip systems is difficult for the rate-independent crystal plasticity. To address this challenge, Bishop and Hill proposed the principle of maximum work [54]. Still, this principle does not alleviate the non-uniqueness in the solution in many cases.

2.2. Rate-dependent onset of slip criterion

The solution to the non-uniqueness problem is found in the field of rate-dependent crystal plasticity and the flow rule for single-crystal visco-plasticity it employs [43,45,55]. The flow rule uses a power-law form to relate the imposed resolved shear stress on the dislocation slip system s to its shear rate, as expressed in Eq. (1). The chief advantage of this flow rule is that it guarantees a unique solution. It leads to a well-posed system of equations when solving for the number of active slip systems needed to determine the strain rate of the crystal, $\dot{\epsilon}_{vp}^c = \sum_s \dot{\gamma}^s \mathbf{m}^{sc}$, and for the deviatoric stress state σ'^c , which consists of five independent stress components.

As the name suggests, this criterion is rate-dependent. For constant τ_c^s , this slip criterion introduces a rate-sensitive material response that scales inversely with n . Fig. 1 shows the variation in slip rate according to the visco-plastic flow rule (1) for different n . Clearly the rate sensitivity introduced by Eq. (1) reduces as n increases. Only in the limit $n \rightarrow \infty$, can this visco-plastic flow rule attain rate-independence.

The problem is that the numerical complexity of finding the solution scales with the power-law exponent n and as a consequence, the value of n representative of many materials is difficult to achieve numerically. As mentioned earlier,

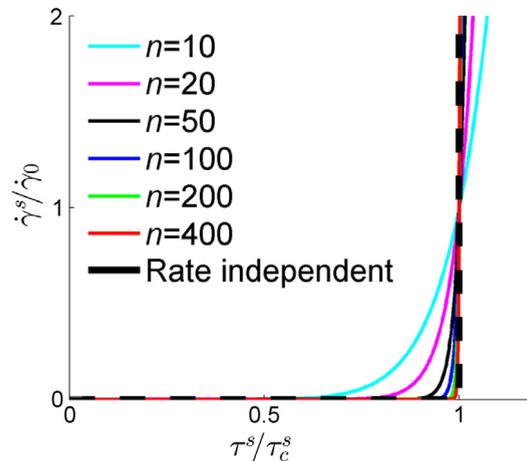


Fig. 1. Rate dependence of crystallographic slip as a function of the power-law exponent n .

for most metals, such as Cu and stainless steel, the value of n is significantly greater than 100 [35,36,44,56]. When n is, for instance, in the range of 1–50, a commonly used set of values in practice today, the Newton–Raphson (NR) solution procedures rarely encounter convergence issues. Modified NR solvers are needed to reach values of $n = 100$. For values of n above 100, however, the use of modified NR solvers is prohibitively computationally intensive as will be shown later in this paper.

Fig. 1 suggests that using numerically friendly values of n (less than 50) that are less than the actual values (100 or greater) would introduce extraneous rate sensitivity. In fact, the further n deviates below the actual value, the more significant the error is.

To confirm, we apply the VPSC model with the visco-plastic flow rule Eq. (1) to a polycrystalline Cu [28]. VPSC is a polycrystal model in which each grain in the polycrystal is treated as a visco-plastic deforming inclusion embedded in a homogeneous effective medium (HEM) [28]. The mechanics of the inclusion problem is solved using a Green’s function approach. The viscoplastic properties of the HEM are calculated by enforcing self-consistency between the macroscopic stress and grain average stresses.

Fig. 2 shows the effect of n on the stress–strain response. In these VPSC simulations, we repeated the simple compression test at different strain rates from 0.001/s to 10/s for a fixed value of τ_c^s . Consequently, no strain rate dependency from τ_c^s is present in these simulations and any rate sensitive response derives from the flow rule and its value of n . In Fig. 2, we show a rate insensitive calculation as a reference,¹ since the expectation is that for higher n , these curves should align closer to this rate insensitive response. As seen in Fig. 2, for $n = 10$, the rate dependency is substantial. As n increases from 10 to 50, the rate dependencies decrease dramatically but are still noticeable. Even for $n = 100$ the curves appear to be close to the rate insensitive response, but yet still exhibit a high strain rate dependencies.

A critical aspect to appreciate is that not only does the computational cost of every call in VPSC increase with n , but so do the difficulties in obtaining a solution. The calculations shown in Fig. 2 for $n = 10$ and 50 were carried out using standard NR schemes. With this approach, however, the solution quickly becomes more difficult beyond $n = 50$. Therefore, the calculations shown for $n = 100$ required a more specialized NR schemes [30,57]. However, even with this advanced scheme, similar stress–strain curves for $n = 400$, which would apply to Cu (as we show later), are still not possible. Solving for the stress given the imposed $\dot{\epsilon}_{vp}^c$ for n higher than 100 results in convergence problems. The non-linear equations become too stiff and prohibitively challenging. Thus achieving values of n corresponding to the rate sensitive behavior of actual materials requires adding an additional solution procedure loop, which incrementally increased n . Here, a solution calculated for a given value of n is used as an initial guess in calculating the next solution for a higher value of n . This incremental increase of n solution procedure is very computationally intensive. However

¹ The rate insensitive response is calculated in VPSC by scaling the shear rates to the norm of the applied strain rate or equivalently by normalizing the strain rate before calling VPSC to calculate the stress. The stress corresponding to a strain rate of unity is always calculated no matter what magnitude the applied strain rate is.

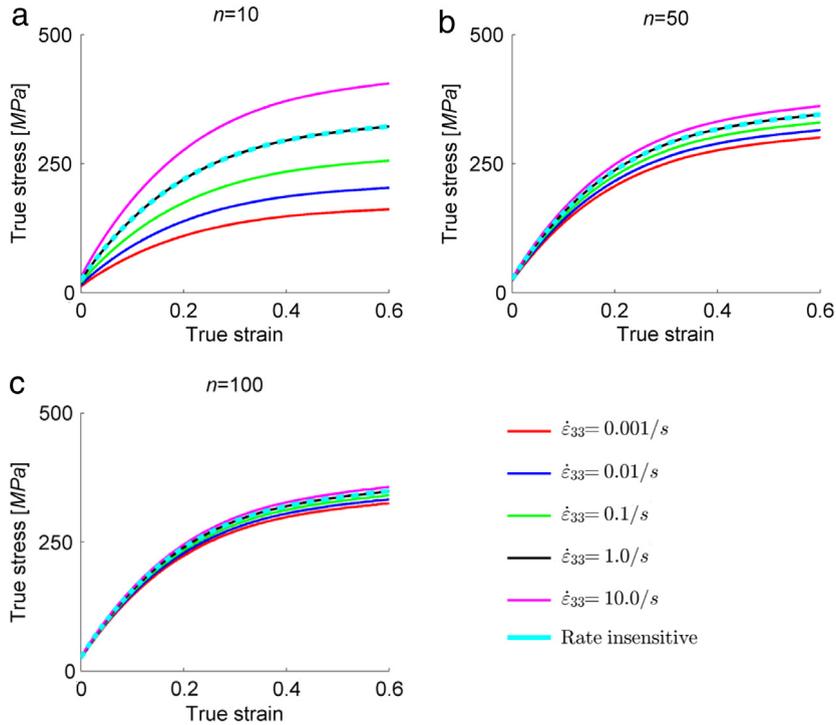


Fig. 2. Effect of n on the room temperature mechanical response of Cu in simple compression as a function of imposed strain rate as indicated in the figure: (a) $n = 10$, (b) $n = 50$, and (c) $n = 100$. The rate insensitive strain rate corresponds to $\dot{\epsilon}_{vp} = 1.0/s$.

and as evident from Fig. 2, using values for n less than needed to model real materials leads to an artificially imposed rate sensitivity.

Introduction of extraneous rate sensitivity via the power-law form Eq. (1) when using non-physically low values of n is a well-recognized problem. One approach, known as the spectral crystal plasticity can circumvent solving the power-law equation and instead evaluates the Fourier series summation of spectral coefficients and Fourier basis [58–61]. The method was found suitable for high-performance computational implementations of crystal plasticity [62,63].

As already mentioned above, another approach consists of incrementally increasing n to a desired value using an additional loop. The loop facilitates that the solution for the lower value of n in the prior iteration over a polycrystal is used as an initial guess for solving for the stress associated with a higher n in the next iteration. Here every crystal comprising an entire polycrystal is solved for a given value of n . The grain stress solution changes with n . To recognize this scaling of the stress, consider scaling the applied strain rate by $\lambda \dot{\epsilon}_{vp}$ while keeping the reference value for the shear rate, $\dot{\gamma}_0$, to be constant. The applied strain rate would result in scaling of the grain stress by $\lambda^{\frac{1}{n}} \sigma'^c$ according to:

$$\lambda \dot{\epsilon}_{vp}^c = \dot{\gamma}_0 \sum_s \mathbf{m}^{sc} \left(\frac{\left| \lambda^{\frac{1}{n}} \sigma'^c \cdot \mathbf{m}^{sc} \right|}{\tau_c^s} \right)^n \text{sign} \left(\lambda^{\frac{1}{n}} \sigma'^c \cdot \mathbf{m}^{sc} \right). \tag{6}$$

Similarly, the overall polycrystal stress would also be scaled, as illustrated in Fig. 2.

Notably this approach permits reaching solutions for n beyond 100; however, it is not computationally efficient and not practical for large scale simulations. The time comparisons will be illustrated later in the paper on the polycrystalline Cu example using this scheme within VPSC. The results will be shown in Fig. 4(a) for up to $n = 400$. To achieve $n = 400$, stable and efficient increments were established to be $n = 50, 100, 150, 200, 250, 300, 350,$ and 400 .

The final approach consists of reducing the rate sensitive response to a rate insensitive one by embedding the norm of an applied strain rate into $\dot{\gamma}_0$ [11,38]. This method involves setting the reference shear rate $\dot{\gamma}_0$, equal to the norm of

the applied macroscopic strain rate, i.e., $\dot{\gamma}_0 = |\dot{\boldsymbol{\epsilon}}_{vp}|$. When $\dot{\boldsymbol{\epsilon}}_{vp}$ is applied, the relation between $\boldsymbol{\sigma}'^c$ and $\dot{\boldsymbol{\epsilon}}_{vp}^c$ follows:

$$\dot{\boldsymbol{\epsilon}}_{vp}^c = |\dot{\boldsymbol{\epsilon}}_{vp}| \sum_s \mathbf{m}^{sc} \left(\frac{|\boldsymbol{\sigma}'^c \cdot \mathbf{m}^{sc}|}{\tau_c^s} \right)^n \text{sign}(\boldsymbol{\sigma}'^c \cdot \mathbf{m}^{sc}). \quad (7)$$

Rate independence is realized when considering another applied strain-rate that scales the given value $\dot{\boldsymbol{\epsilon}}_{vp}$, say by λ . Accordingly, the new rate equation in the grain is given by:

$$\lambda \dot{\boldsymbol{\epsilon}}_{vp}^c = |\lambda \dot{\boldsymbol{\epsilon}}_{vp}| \sum_s \mathbf{m}^{sc} \left(\frac{|\boldsymbol{\sigma}'^c \cdot \mathbf{m}^{sc}|}{\tau_c^s} \right)^n \text{sign}(\boldsymbol{\sigma}'^c \cdot \mathbf{m}^{sc}). \quad (8)$$

Note that λ only changes the magnitude of the applied strain rate and not the sense of loading. Evidently, the stress $\boldsymbol{\sigma}'^c$ will remain unchanged provided that τ_c^s does not change with strain-rate making the response rate independent. Scaling the applied strain rate by $\lambda \dot{\boldsymbol{\epsilon}}_{vp}$ makes the grain strain rates also scale since

$$\dot{\boldsymbol{\epsilon}}_{vp} = \langle \dot{\boldsymbol{\epsilon}}_{vp}^c \rangle \rightarrow \lambda \dot{\boldsymbol{\epsilon}}_{vp} = \langle \lambda \dot{\boldsymbol{\epsilon}}_{vp}^c \rangle. \quad (9)$$

Evidently, the grain stress and the overall polycrystal stress will not scale as long as $\dot{\gamma}_0 = |\lambda \dot{\boldsymbol{\epsilon}}_{vp}|$.

It is worth mentioning that this last approach may introduce a problem if one were to implement it into finite elements [64–68]. According to this approach, the deviatoric stress, $\boldsymbol{\sigma}'^c$, is no longer a function of $|\dot{\boldsymbol{\epsilon}}_{vp}|$, but a function of four independent components of the normalized visco-plastic strain rate. Thus, the solution for the five-component deviatoric stress, $\boldsymbol{\sigma}'^c$, contains five *dependent* deviatoric stress components. Consequently, the Cauchy stress representing a hyper-surface in six-dimensional stress space required by Abaqus will only have five, not six, independent components. Difficulties could arise when attempting to solve for the Cauchy stress within the finite element framework.

3. The k -modification (k -mod) method

In light of the issues introduced by the above methods, it is clear that removing the superfluous rate sensitivity from the rate-dependent criterion that is introduced with inaccurately low values of n is a long-standing problem still in need of a solution. In this work, we propose a novel method for solution that allows for a broad range of values for rate sensitivity, while being computationally efficient.

The method appropriately modifies the applied strain rate at the grain level. We begin by defining a rate-sensitive macroscopic constitutive function, \mathbf{g} , for relating the macroscopic stress, $\boldsymbol{\sigma}'$, and applied macroscopic strain rate, $\dot{\boldsymbol{\epsilon}}_{vp}^{app}$, via

$$\boldsymbol{\sigma}' = \mathbf{g}(\dot{\boldsymbol{\epsilon}}_{vp}^{app}). \quad (10)$$

The key idea in the second step involves adjusting the applied strain rate before evaluating the visco-plastic constitutive function. Specifically in place of the original rate $\dot{\boldsymbol{\epsilon}}_{vp}^{app}$, we use a modified strain rate, $\dot{\boldsymbol{\epsilon}}_{vp}$, whose norm is the $(k + 1)$ th root of $\dot{\boldsymbol{\epsilon}}_{vp}^{app}$, i.e.,

$$\dot{\boldsymbol{\epsilon}}_{vp} = \frac{\dot{\boldsymbol{\epsilon}}_{vp}^{app}}{|\dot{\boldsymbol{\epsilon}}_{vp}^{app}|} |\dot{\boldsymbol{\epsilon}}_{vp}^{app}|^{\frac{1}{k+1}}. \quad (11)$$

Note that norms and powers apply only to the values and not to the units. The inverse relationship is given by:

$$\dot{\boldsymbol{\epsilon}}_{vp}^{app} = \dot{\boldsymbol{\epsilon}}_{vp} |\dot{\boldsymbol{\epsilon}}_{vp}|^k. \quad (12)$$

The corresponding macroscopic visco-plastic constitutive function is:

$$\mathbf{g}(\dot{\boldsymbol{\epsilon}}_{vp} (\dot{\boldsymbol{\epsilon}}_{vp}^{app})) = \mathbf{g} \left(\frac{\dot{\boldsymbol{\epsilon}}_{vp}^{app}}{|\dot{\boldsymbol{\epsilon}}_{vp}^{app}|} |\dot{\boldsymbol{\epsilon}}_{vp}^{app}|^{\frac{1}{k+1}} \right) = \mathbf{f}(\dot{\boldsymbol{\epsilon}}_{vp}^{app}). \quad (13)$$

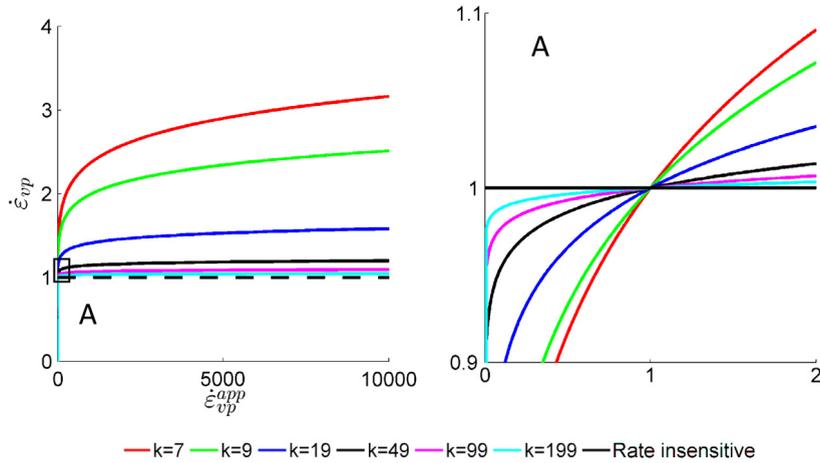


Fig. 3. Effect of k on relaxing the strain rate dependence of grain level response.

The macroscopic stress is evaluated using a different constitutive relationship, $\mathbf{f} = \mathbf{g} \circ \dot{\epsilon}_{vp}$, with the applied strain rate, $\dot{\epsilon}_{vp}^{app}$, which is less strain rate sensitive than the original relationship \mathbf{g} in Eq. (10), provided that $k > 0$. The sign ‘ \circ ’ denotes the composition.

Fig. 3 illustrates Eq. (11), where $\dot{\epsilon}_{vp} = |\dot{\epsilon}_{vp}|$ is calculated as a function of $\dot{\epsilon}_{vp}^{app} = |\dot{\epsilon}_{vp}^{app}|$ up to a value of 10,000 /s and k up to a value of 199. These particular calculations are performed for a macroscopic simple compression test but the plot would look the same for any imposed boundary conditions. The analogy of Eq. (1) at the slip system level (Fig. 1) and Eq. (11) at the grain level (Fig. 3) can be observed. As k increases, the solution for $\dot{\epsilon}_{vp}$ approaches the rate independent grain level response, which is another way of obtaining Eq. (8). The full agreement between Eq. (8), i.e. the strain rate insensitive scaling, and the k -mod will be the case when $k \rightarrow \infty$. Here, the applied strain rate would be a unity. The effect of k on scaling the stress will be explained shortly and illustrated in Fig. 4.

As before, suppose the strain rate is altered to $\lambda \dot{\epsilon}_{vp}^{app}$. As a result, the k -mod strain rate $\dot{\epsilon}_{vp}$ changes to $\lambda^{\frac{1}{k+1}} \dot{\epsilon}_{vp}$. The grain strain rate as well as the resulting homogenized polycrystal strain rate becomes:

$$\dot{\epsilon}_{vp} = \langle \dot{\epsilon}_{vp}^c \rangle \rightarrow \lambda^{\frac{1}{k+1}} \dot{\epsilon}_{vp} = \langle \lambda^{\frac{1}{k+1}} \dot{\epsilon}_{vp}^c \rangle, \tag{14}$$

where

$$\lambda^{\frac{1}{k+1}} \dot{\epsilon}_{vp}^c = \dot{\gamma}_0 \sum_s \mathbf{m}^{sc} \left(\frac{|\mathbf{m}^{sc} \cdot \lambda^{\frac{1}{k+1}} \boldsymbol{\sigma}'^c|}{\boldsymbol{\tau}_c^s} \right)^n \text{sign} \left(\mathbf{m}^{sc} \cdot \lambda^{\frac{1}{k+1}} \boldsymbol{\sigma}'^c \right). \tag{15}$$

Eq. (15) shows that the grain stresses and as a result the homogenized macroscopic stress scale according to:

$$\boldsymbol{\sigma}' = \langle \boldsymbol{\sigma}'^c \rangle \rightarrow \lambda^{\frac{1}{(k+1)n}} \boldsymbol{\sigma}' = \left\langle \frac{1}{(k+1)n} \boldsymbol{\sigma}'^c \right\rangle. \tag{16}$$

The strain rates within the grains scale by $\frac{|\dot{\epsilon}_{vp}^{app}|}{|\dot{\epsilon}_{vp}^{app}|^{\frac{1}{k+1}}}$ to ensure that they correspond to $\dot{\epsilon}_{vp}^{app}$, which is evident considering the following:

$$\langle \dot{\epsilon}_{vp}^c \rangle = \dot{\epsilon}_{vp} \rightarrow \langle \dot{\epsilon}_{vp}^c \rangle = \frac{\dot{\epsilon}_{vp}^{app}}{|\dot{\epsilon}_{vp}^{app}|} |\dot{\epsilon}_{vp}^{app}|^{\frac{1}{k+1}} \rightarrow \left\langle \dot{\epsilon}_{vp}^c \frac{|\dot{\epsilon}_{vp}^{app}|}{|\dot{\epsilon}_{vp}^{app}|^{\frac{1}{k+1}}} \right\rangle = \dot{\epsilon}_{vp}^{app}. \tag{17}$$

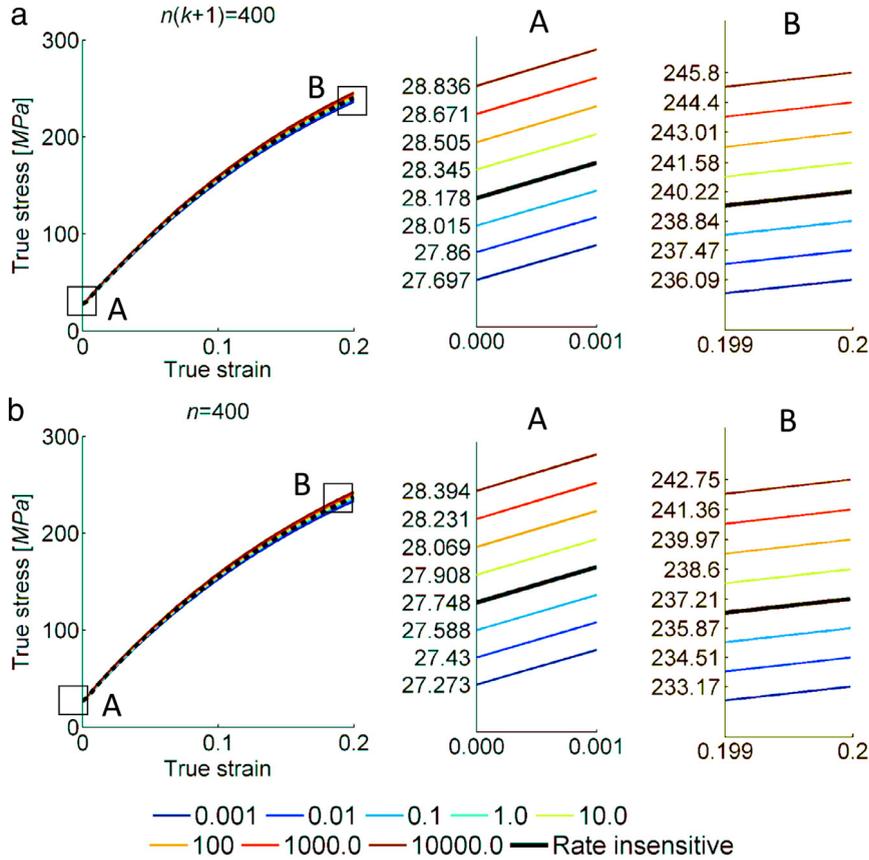


Fig. 4. Relaxing the power-law imposed strain-rate sensitivity of the mechanical response of Cu in simple compression as a function of imposed strain rate $\dot{\epsilon} = |\dot{\epsilon}_{vp}|$ as indicated in the figure by: (a) a combination of $n = 50$ and $k + 1 = 8$ and (b) solely $n = 400$. Note that the scaling in stress is identical i.e. if the applied strain rate increases 10 times then stress increase according to $10^{\frac{1}{400}} \sigma'$ in both (a) and (b).

Finally, the scaling of $\dot{\epsilon}_{vp}^c$ reflects on the shear rates as follows:

$$\dot{\epsilon}_{vp}^c \frac{|\dot{\epsilon}_{vp}^{app}|}{|\dot{\epsilon}_{vp}^{app}|^{\frac{1}{k+1}}} = \sum_s \mathbf{m}^s \left(\dot{\gamma}^s \frac{|\dot{\epsilon}_{vp}^{app}|}{|\dot{\epsilon}_{vp}^{app}|^{\frac{1}{k+1}}} \right). \tag{18}$$

From Eq. (15), we see that the rate sensitivity is now characterized by both the power-law exponent n and the additional exponent k . The power-law exponent is now multiplied by $k + 1$, which has the effect of decreasing the overall rate sensitivity effect, provided again that $k > 0$. The grain and macroscopic stresses change by a factor of $\lambda^{\frac{1}{(k+1)n}}$. Therefore the desired effect is elegantly obtained.

We note that the scaling in Eqs. (6) and (15) is the same. For instance, we can achieve an exponent of 400, either by $n = 400$ and $k = 0$ in Eq. (6) or with $n = 50$ and $k = 7$ in Eq. (15), to give $(k + 1)n = 400$. As a result, any value of a strain rate sensitivity exponent as the material property can be realized using a combination of n and k . It is convenient to fix n since it is already incorporated in Eq. (15) and only vary k , thus only Eq. (15) is used to achieve any desired strain rate sensitivity exponent. Fig. 4 illustrates a particular example comparing the stress–strain response for the same test at different strain rates using the slip system level power-law for $n = 400$ (obtained by the incremental n approach) and the combination of slip system level power-law and grain level k -mod power-law method for $n = 50$ and $k + 1 = 8$, which provides a combined power-law exponent of $(k + 1)n = 400$ as a stress modifier. The actual stress values from the two approaches in Fig. 4(a) and (b) differ only slightly, within 1% or 2%. This difference is expected due to numerically solving the slip system power law with a different n value for a given applied strain rate.

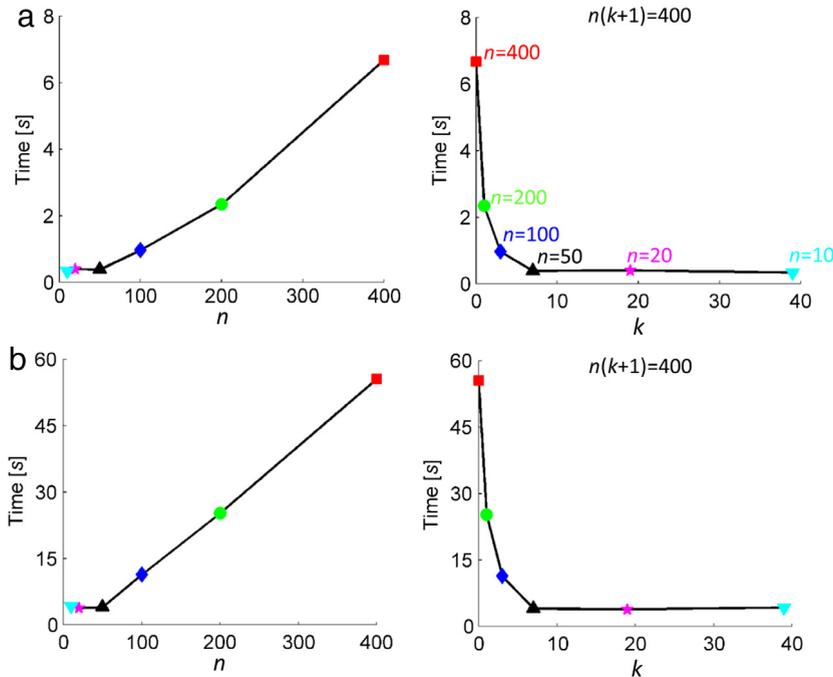


Fig. 5. Computational time involved in solving the visco-plastic equation in simple compression for 400 randomly oriented crystals in (a) Taylor-type and (b) self-consistent (VPSC) homogenizations. On the left is shown increase in computational time as a function of n . Note that the solutions for $n > 50$ is obtained using the slip system level power-law solution methodology with incrementing n in increments of 50. On the right is shown decrease in computational time involved in solving $n(k + 1) = 400$ case where n and k are varied as indicated in the figure. Note here that a compromise of the time involved, accuracy, and numerical stability is achieved using $n = 50$ and $k + 1 = 8$.

Importantly, the scaling between stress values with applied strain rates is exactly the same and equal to $\lambda^{\frac{1}{400}} \sigma'$ for both methods as guaranteed by $\lambda^{\frac{1}{n}} \sigma'$ and $\lambda^{\frac{1}{(k+1)n}} \sigma'$, respectively. It should be noted that slip system power-law rate sensitivity characterized by n enters the VPSC solution procedure for stress given the applied strain rate $\dot{\epsilon}_{vp}$. Due to the k -mod power-law characterized by k , which is embedded within adjusted $\dot{\epsilon}_{vp}$, the final strain rate sensitive grain level stress as well as the overall polycrystal stress is determined by both k and n .

Ultimately, we aim to reduce the rate sensitivity as much as needed without significantly increasing computation time. In this regard, the significant advantage of the k -mod method in Fig. 4(a) is that it requires substantially less computation time. Essentially, it does not add any time to solving the slip system power-law with a given value of n . The computational time to solve for the stress given the strain rate increases with n , but remains constant with increase in k . To demonstrate this, we return to the same example as shown in Fig. 4 and compare the computation time when using the incremental n approach and the k -mod method. Fig. 5 shows the results for two types of polycrystal models, the full constraints Taylor model (Fig. 5(a)) and as before the VPSC model (Fig. 5(b)). The subfigures on the left show the computation time (in seconds, for simple compression up to -0.2 compressive strain) as a function of n , up to 400, using only the slip system level power-law. As shown, the computation time exhibits a nearly linear increase with n . Clearly, obtaining a solution only via the slip system level power-law for $n > 100$ would be computationally intensive and not practical. The times are significantly longer in the VPSC scheme versus the Taylor scheme since for every increment in n (say from $n = 100$ to $n = 150$) there are several self-consistent iterations to be solved over the polycrystal. Therefore, the time increases as a product of the number of self-consistent iterations and increments in n .

The figures on the right present the computation times for a fixed $(k + 1)n = 400$ i.e. $m = 0.0025$. For even low values of k , such as 1 and 3, the computation time has vastly improved over the slip-system level power-law alone for the same exponent value of 400. For both polycrystal models, Taylor and VPSC, the best compromise in computation time, accuracy, and numerical stability is achieved using $n \leq 50$. The use of as high as possible n values affects the slip

system rate sensitivity. However, too high n values result in numerical instabilities and increase the time. Therefore a good combination of n and k for achieving the strain rate exponent corresponding to $m = 0.0025$ is for example $n = 50$ and $k + 1 = 8$. More generally, these results clearly show that using k -mod method can cost potentially much less time than the slip-system level scheme alone. Use of the k -mod method is especially advantageous for VPSC since the solution procedure needed to achieve self-consistency involves substantially many more iterations.

It is worth noting that low values of n can cause the slip systems to be active over a relatively wide range of stresses, making the results smooth with respect to a change in stress. In contrast, high values of n bring the resolved shear stress closer to the slip resistance for each active system making the range of stresses to reduce and correspond to a particular slip system. In addition to making the activation threshold sharper, it also makes the direction of strain rate very sensitive to changes in stress. While the magnitude of strain rate is defined by both n and k , the increase in k does not affect the relative contribution of deformation systems that are active but only affects the scaling of the norm of strain rate with the norm of stress. As a result, the direction of strain rate is defined solely by n meaning that the unrealistic smoothing associated with lower values of n can be present in the k -modification approach. However smoothing is not expected to cause any appreciable differences in the response and especially in the macroscopic-level response, as long a sufficiently high value of n is used.

4. Discussion

With the k -mod method developed here, grain level strain rate-sensitivity exponents can span a much broader range than before with prior methods. Advantageously as low values of rate sensitivity m as necessary can be reached, enabling the consideration of the true rate sensitivity of materials within crystal plasticity frameworks, without increasing computation time. Inaccurately low values of n not only are unconnected with the actual material value, but can also introduce an unwanted relationship between the rate-sensitive activation stresses τ_c and the rate-sensitive macroscopic response. With the k -mod method, the rate sensitivity embedded in the evolution of the activation stresses τ_c can be propagated faithfully through the length and time scales of a multiscale materials model and the way it affects the macroscopic response can be analyzed.

To demonstrate the utility of the model, we incorporate the k -mod method into the polycrystal plasticity model VPSC and apply it to polycrystalline Cu (0.9999 purity). The experimental data used came from Follansbee and Kocks [10,35], where the material was tested over a wide range of strain rates from 10^{-4} /s to 10^4 /s. Over this range, they sought to measure the flow stresses corresponding to a fixed microstructural state. This effort involves analyzing the change in the macroscopic stress with strain rate for material possessing the same internal defect state. In terms of the model, this translates to holding τ_c fixed while the applied strain rate varies. In their work, this analysis was repeated for three microstructural states, corresponding to three different τ_c . The VPSC model was calibrated to the experimental data and the following values of τ_c were obtained: 67, 85, and 103 MPa. In Fig. 6, we compare our model predictions with their data for different values of k with $n = 50$. The comparison suggests that for all three microstructural states, $n = 50$, $k = 7$ provides the best agreement, giving an exponent of $(k + 1)n = 400$ or a strain rate sensitivity of 0.0025.

This application to polycrystalline Cu can be considered a stringent test of the k -mod method, since this metal exhibited relatively low rate sensitivity. This case would be extremely difficult to model with a standard polycrystal model utilizing the power-law visco-plasticity flow rule. With the k -mod method, a single computational call for the stress–strain solution negligibly adds to the computation time involved at the grain level and thus does not appreciably increase the overall polycrystal calculations. Such computational efficiency would have been impossible to achieve with currently available methods.

With the appropriate value of the exponent in hand, we can now model the stress–strain response of Cu. The value of τ_c evolves with straining at a rate that depends on temperature and strain rate. The evolution law (or hardening law) for $\tau_c(\varepsilon, T)$ is taken from [69–72] and used in VPSC. The parameters for the hardening law are provided in Table 1 and include the initial friction stress τ_0 , the trapping rate coefficient k_1 , the activation barrier for dynamic recovery g , a drag stress D , dislocation interaction coefficient χ_0 , and substructure development coefficient q . We refer the reader to [72] for more details on the hardening model.

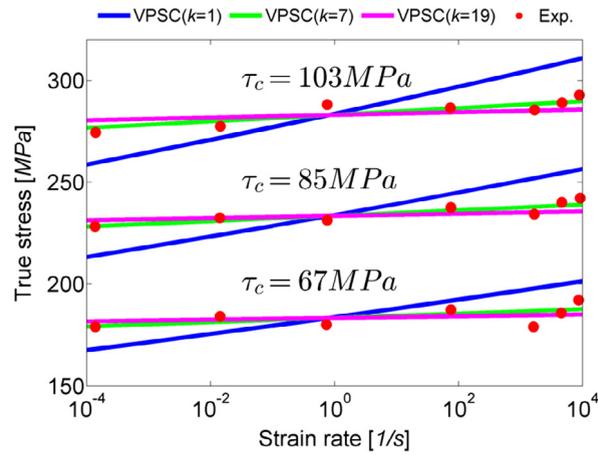


Fig. 6. Achieving the strain-rate sensitivity of Cu using the combination of slip system power-law flow rule and grain scale k -mod power-law method. The data measured in simple compression at the three pre-strain levels was taken from [35]. The strain rate sensitivity exponent able to fit the experimental data is determined to be 0.0025. It is achieved through a combination of $n = 50$ and $k = 7$. The starting texture was 400 randomly oriented grains deformed in one deformation step as a function of strain rate with the three different values of τ_c .

Table 1
Model parameters for evolution of slip resistance for Cu.

τ_0 [MPa]	k_1 [m^{-1}]	g	D [MPa]	q	χ_0
10.1	2.2×10^8	0.0167	800	$0.14/\dot{\epsilon}^{0.55}$	0.81

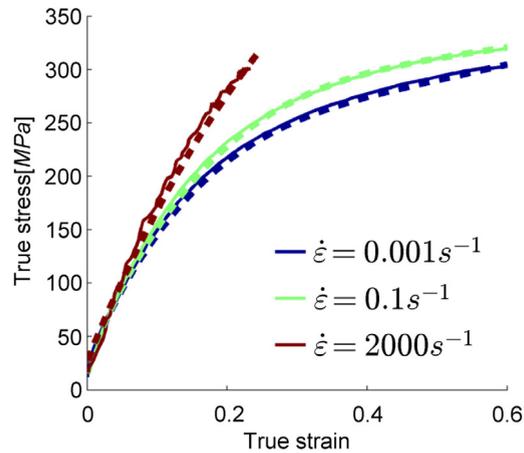


Fig. 7. Measured and predicted true stress-true strain response for Cu achieved using of $n = 50$ and $k = 7$ and the evolution law for slip resistance as a function of applied strain rate.

Fig. 7 compares the measured and calculated stress–strain response using $(k + 1)n = 400$. As shown, the model, using the same set of material parameters in Table 1, is able to capture all three responses and hence the rate sensitive material behavior.

5. Conclusions

In this article, we develop a novel method that enables the use of true strain rate sensitivity exponents for polycrystals within crystal visco-plasticity without increasing computation time involved in polycrystal simulations. While values of n associated with true visco-plastic properties for polycrystalline metals can range from 10^2 to 10^3 , current methods in crystal visco-plasticity are numerically limited to values of n less or equal to 100. Additionally, the method facilitates true separation of strain rate-sensitivity embedded in the evolution of the activation stress due to microstructural evolution from the constant structure rate sensitivity embedded in the exponent. To demonstrate the utility of the new method, called the k -modification method, calculations are performed for polycrystalline pure Cu, which has a relatively low strain rate sensitivity of $m = 0.0025$ or equivalently a high exponent value of $n = 400$. Excellent agreement with experimental measurement demonstrates that this development is the first time a polycrystal visco-plasticity model implementation able to represent thermally activated dislocation motion across length scales in quantitative agreement with a wide range of experimental conditions. This method can be used to model the strain rate-sensitive behavior for a wide range of metals.

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