Crystal plasticity within small strain theory

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The purpose of this post is to briefly introduce the basic concepts of a simple crystal plasticity model formulation. More advanced topics will be presented later.

0.1 Introduction

The aim of a crystal plasticity model is to integrate the symmetries of the crystal lattice into the formulation for plastic flow. This framework acknowledges individual slip systems, but instead of focusing on individual dislocations, it considers them on an average scale through densities. The crystal plasticity framework is well-suited for modeling the behavior of single crystals and polycrystalline aggregates, where explicit representation of individual grains is employed.

In this section, we lay the foundations of a straightforward crystal plasticity model based on the assumptions of the small strain theory.

0.2 Kinematics

According to the small strain theory, the kinematics of deformation can be described by decomposing the total strain **rate** into elastic and plastic components, using an additive approach.

$$\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}^e + \dot{\boldsymbol{\varepsilon}}^p$$

where the strain measure is defined by:

$$\boldsymbol{\varepsilon} = \frac{1}{2}\left(\boldsymbol{\nabla}\boldsymbol{u} + (\boldsymbol{\nabla}\boldsymbol{u})^T\right) \tag{1}$$

Here $\boldsymbol{u}$ is the displacement field and $\boldsymbol{\nabla}$ is the divergence operator.

The rate of plastic strain is proportional to dislocation slip on individual slip planes α

$$\dot{\boldsymbol{\varepsilon}}^p = \sum_\alpha \dot{\gamma}^\alpha \left(\vec{m}^\alpha \odot \vec{n}^\alpha\right) \operatorname{sign}(\tau^\alpha) \tag{2}$$

where the notation $\odot$ is used for the symmetric tensor product: $\vec{m}_0^\alpha \odot \vec{n}^\alpha = \frac{1}{2}\left[\vec{m}^\alpha \otimes \vec{n}^\alpha + \vec{n}^\alpha \otimes \vec{m}_0^\alpha\right]$.

The slip systems for the FCC crystal lattice are provided in the table below:

0.3 Hardening law

$$\dot{s}^\alpha = \sum_\beta h^{\alpha\beta} |\dot{\gamma}^\beta|$$

For the case of no hardening, $h^{\alpha\beta} = 0$. (Taylor, 1983) proposed $h^{\alpha\beta} = h$, and (Pierce et al., 1983)

$$h^{\alpha\beta} = h(\gamma)\left[q + (1-q)\delta^{\alpha\beta}\right]$$

0.4 Flow rule

0.4.1 Rate-independent formulation (yield surface)

In the rate-independent formulation one needs to define a yield surface. The amount of slip will then be calculated from the consistency condition. Only some of the slip systems will be active.

We will consider the following yield surface:

$$|\tau^\alpha| = s^\alpha \tag{3}$$

and during the plastic flow, the active slip systems must satisfy the consistency condition

$$|\dot{\tau}^\alpha| = \dot{s}^\alpha \tag{4}$$

The resolved shear stress is calculated following:

$$\tau^\alpha = \boldsymbol{\sigma} : \vec{m}^\alpha \odot \vec{n}^\alpha \operatorname{sign}(\tau^\alpha)$$

This is also called the associated flow rule where all components of stress do work, unlike in the more complex case of non-Schmidt effects where some stress components only distort the core of dislocations (especially in BCC metals).

Substituting the derived equations into the consistency condition, we arrive to the following:

$$\begin{gathered} \dot{\boldsymbol{\sigma}} : \vec{m}^\alpha \odot \vec{n}^\alpha \operatorname{sign}(\tau^\alpha) = \sum_\beta h^{\alpha\beta} |\dot{\gamma}^\beta| \\ \left[\mathcal{C} : \dot{\varepsilon} - \operatorname{sign}(\tau^\beta)\mathcal{C} : \sum_\beta \dot{\gamma}^\beta \vec{m}^\beta \odot \vec{n}^\beta\right] : \vec{m}^\alpha \odot \vec{n}^\alpha \operatorname{sign}(\tau^\alpha) = \sum_\beta h^{\alpha\beta} |\dot{\gamma}^\beta| \end{gathered} \tag{5}$$

We can rewrite these equations into a system of linear equations:

$$\left[h^{\alpha\beta} + \text{sign}(\tau^\alpha)\text{sign}(\tau^\beta)\vec{m}^\alpha \odot \vec{n}^\alpha : \mathcal{C} : \vec{m}^\beta \odot \vec{n}^\beta\right]\dot{\gamma}^\beta = \text{sign}(\tau^\beta)\vec{m}^\alpha \odot \vec{n}^\alpha : C : \dot{\boldsymbol{\varepsilon}} \tag{6}$$

therefore

$$A^{\alpha\beta}\dot{\gamma}^\beta = b^\alpha \tag{7}$$

Noticed that we have removed the absolute value from the rate of shearing, and as we proceed with solving these equations, we will only consider the case for which $\dot{\gamma}^\beta > 0$.

Since various combinations of slip systems and slip shearing rates could result in the same deformation, the solution is not unique. To overcome this issues, we may select such result which of of the possible combinations will yield the least amount of energy. The system of equations can be efficiently solved using the singular value decomposition [Kothari].

Thus for a given strain rate $\Delta\boldsymbol{\varepsilon}/\Delta t$, the increment in shearing can be calculated $\Delta\gamma^\alpha$.

0.4.2 Rate-dependent formulation (kinetics of dislocation slip)

In the rate-dependent formulation, all slip systems are always active although the small rate of slip of some slip systems may be perceived as inactivity. The kinetic law governing the rate of shear can be of a very general form:

$$\dot{\gamma}^\alpha = f(\text{stress, material state, temperature, ...}).$$

The kinetic law can be of phenomenological, physical, or strain gradient nature. The most commonly used is an empirical power law

$$\dot{\gamma}^\alpha = A^\alpha\left(\tau^\alpha\right)^m$$

While this law is easy to implement, it is purely empirical temperature independent and may be valid only within certain physical limits. The most common form of the power law is [**?**]:

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

Unable to capture the physical limits of dislocation velocities and temperature effects, the power law is primarily used as a numerical device due to its simplicity fitted to be valid in a certain specific range of loading conditions.

A more physical model of thermally activated slip is based on the Arrhenius-type of equations [**?**], [**?**]:

$$\dot{\gamma}^\alpha = \begin{cases} 0 & \text{if} \quad \tau_{\text{eff}}^\alpha \le 0 \\ \dot{\gamma}_0^\alpha \exp\left\{-\frac{\Delta G}{kT}\right\} & \text{if} \quad \tau_{\text{eff}}^\alpha > 0 \end{cases} \tag{8}$$

where ΔG is the energy barrier needed to be overcome by thermal fluctuations:

$$\Delta G = G_0\left[1 - \left(\frac{\tau_{\text{eff}}^\alpha}{s_t^\alpha}\right)^p\right]^q \tag{9}$$

and $\tau_{\text{eff}}^\alpha = |\tau^\alpha| - s_a^\alpha$ is the effective stress.

The coefficients p and q represent the shape of the barriers opposing the dislocation motion.

For more interested readers, another form of the activation enthalpy was presented by [**?**]

To find the solution in the rate-dependent case seems now more straightforward as the equations can be easily discretized. For the explicit discretization,

$$\Delta\gamma^{\alpha} = \Delta t \dot{\gamma}_0^{\alpha} \left| \frac{\tau^{\alpha}(t)}{s^{\alpha}(t)} \right| \mathrm{sign}(\tau^{\alpha}(t)) \tag{10}$$

0.5 Analytical solutions

For simple case, it may be possible to derive analytical or semi-analytical solutions.

Consider a single crystal under [001], [110], and [111] orientation. These are the points of the stereographic triangle, and for these three specific case, 8, 4, and 6 slip systems will be active with exact the same amount of slip on all of them. For illustration, we consider the [001] case. Furthermore, we assume isotropic elastic material properties defined by Young's modulus E and Poisson's ratio ν.

(Taylor, 1983)

(Pierce et al., 1983)