Dislocation-density based crystal plasticity finite element model

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This short manuscript highlights the basic formulation and key algorithm of the dislocation-density based crystal plasticity finite element (DD-CPFE) model. This work is based on our previous DDEHM model. The idea is to employ the constitutive update scheme from DDEHM model for each integration point of the microstructure. Comparing with the DDEHM model, the largest difference of the DD-CPFE model is the stress update.

For small deformation, the stress-strain relation (in rate form) can be written as:

$$\dot{\sigma}_{ij} = L_{ijkl}(\dot{\bar{\epsilon}}_{kl} - \dot{\mu}_{kl}) \tag{1}$$

where the $\bar{\boldsymbol{\epsilon}}$ is the total strain and $\boldsymbol{\mu}$ is the plastic strain.

The plastic strain, which is contributed by crystal plasticity, is expressed as:

$$\dot{\mu}_{ij} = \sum_{s=1}^{N} \dot{\gamma}^s Z_{ij}^s \tag{2}$$

where N is the number of slip systems, $\dot{\gamma}^s$ is the slip rate of s^{th} slip system and $\boldsymbol{Z}$ is the Schmid's tensor.

Eq.(1) and (2) is the constitutive equation in a general sense. To complete the description, one can refer to DDEHM model, where the expression for $\dot{\gamma}^s$ is presented.

Next, we will introduce the algorithm for stress update and algorithmic moduli. The residual of stress update is written as:

$$\Phi_I = \frac{{}_{l+1}\sigma_I - {}_{l}\,\sigma_I}{{}_{l+1}\Delta t} - L_{IJ}\left(\frac{{}_{l+1}\epsilon_J - {}_{l}\,\epsilon_J}{{}_{l+1}\Delta t} - \dot{\mu}_J\right) \tag{3}$$

The corresponding Jacobian is defined as:

$$\frac{\partial \Phi_I}{\partial \sigma_J} = \frac{1}{{}_{l+1}\Delta t}\delta_{IK} + L_{IJ}\frac{\partial \dot{\mu}_J}{\partial \sigma_K} \tag{4}$$

Note that in Eq.(3) and (4), the expression for $\dot{\mu}_J$ and $\frac{\partial \dot{\mu}_J}{\partial \sigma_K}$ can be found in DDEHM model.

The plastic moduli can be computed by taking the derivative of the residual with respect to the strain as:

$$\frac{\partial_{l+1}\sigma_I}{\partial_{l+1}\epsilon_J} = L_{IK}\left(\delta_{KJ} - \frac{\partial_{l+1}\dot{\mu}_K}{\partial_{l+1}\bar{\epsilon}_J}\right)_{l+1}\Delta t \tag{5}$$

Utilizing chain rule, Eq. (5) can be written as:

$$\left(\frac{1}{{}_{l+1}\Delta t}\delta_{IP} + L_{IK}\frac{\partial_{l+1}\dot{\mu}_K}{\partial_{l+1}\tau}\frac{\partial_{l+1}\tau}{\partial_{l+1}\sigma_P}\right)\frac{\partial_{l+1}\sigma_P}{\partial_{l+1}\bar{\epsilon}_J} = \frac{L_{IJ}}{{}_{l+1}\Delta t} \tag{6}$$

which contains a linear system of equation to be solved for the plastic moduli.

The proposed DD-CPFE model was verified against DDEHM model for a quasi-2D microstructure containing 9 grains (Fig 1). The stress-strain curve shows a 5% error (Fig 2).

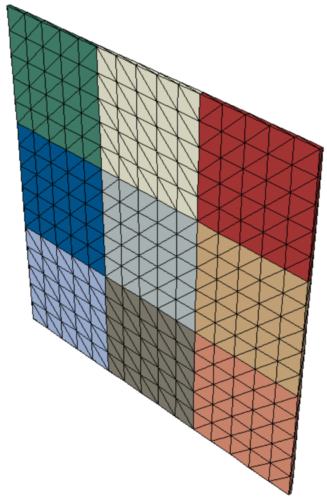

Figure 1: A quasi-2D microstructure containing nine grains

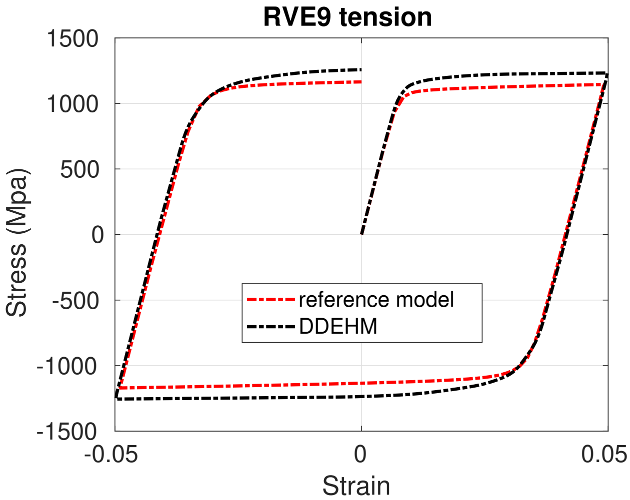

Figure 2: Engineering stress-strain curves of DD-CPFE and DDEHM models