Crystal plasticity subroutine for ABAQUS (UMAT)

Subroutine version 5.3

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0. Release notes (from version 5)

-- EXP MAP and DEXP MAP are suppressed (linear approach)
-- Includes more general symmetry of stiffness matrix (orthotropic)
-- write of messages supressed
-- Works (generally) under parallel in all ABQ versions (6.7-6.11)
-- Now the former file subroutines_v4.f is included in file
-- Voce Hardening law included.

1. Introduction

The subroutine developed is a constitutive model of crystal plasticity for the implicit FE code ABAQUS [1]. It is programed in finite strains (using hyperelastic approach) and based on the multiplicative decomposition of plastic strain.

2. Description of the constitutive equation

A brief summary of the model equations is

The decomposition of the deformation gradient, ***F***, into its elastic F^e and plastic part F^p is assumed [2-6]

$$F = F^e F^p \quad . \qquad (1)$$

Using the definition of the velocity gradient, $L \equiv \nabla_x v = \dot{F} F^{-1}$, expression (1) leads to the additive decomposition of L as

$$L = L^e + F^e L^p F^{e-1} \qquad (2)$$

being L^e and L^p the elastic and the plastic velocity gradients, respectively. If plastic deformation takes place along multiple slip systems, L^p is defined as the sum of the shear rate, $\dot{\gamma}$, for each slip system, α according to:

$$L^p = \sum_{\alpha} \dot{\gamma}^{\alpha} \left(s^{\alpha} \otimes m^{\alpha} \right) \qquad (3)$$

where s^{α} and m^{α} stand, respectively, for the unit vectors in the slip direction and normal to the slip plane in the reference configuration.

The crystal is assumed to behave as an elasto-viscoplastic solid in which the plastic slip rate for a given slip system, follows a power-law dependency,

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_o \left(\frac{\left| \tau^{\alpha} \right|}{g^{\alpha}} \right)^{\frac{1}{m}} sgn\left(\tau^{\alpha} \right) \qquad (4)$$

where $\dot{\gamma}_o$ is a reference shear strain rate, g^{α} the critical shear stress on the slip system, and m the rate-sensitivity exponent [7]. τ^{α} stands for to the resolved shear stress on the α slip system, which is obtained as the projection of the Kirchoff stress on that system according to

$$\tau^{\alpha} = C \left[\left(F_{\square}^{e\,T} F_{\square}^{e} \right)^{\frac{1}{2}} - I \right] : s^{\alpha} \otimes m^{\alpha} \qquad (5)$$

where C represents the elastic stiffness tensor of the crystal.

The evolution of the critical shear stress, g^{α} , for a given slip system, α , is obtained using the classical hardening model of Asaro and Needleman , which defines the current slip resistance as:

$$\dot{g}^{\alpha} = \sum_{\beta} q_{\alpha\beta} h\left(\Gamma \right) \dot{\gamma}_{\beta} \qquad (6)$$

where $q_{\alpha\beta}$ with $\alpha=\beta$ and $\alpha\neq\beta$ are the self- and the latent-hardening coefficients, respectively.[22] *h* is referred to as the hardening modulus and two approaches are followed here

(a) Assaro-Needleman hardening law (providing a saturation law only valid for stage I)

$$h(\Gamma)=h_0 sech\left|\frac{h_0\Gamma}{\tau_s-\tau_0}\right|^2 \qquad (7a)$$

(b) Voce model adapted by Tomé to single crystals (providing the possibility of stage II)

$$h(\Gamma)=h_0+\left(h_0-h_1+\frac{h_0 h_1}{\tau_s}\Gamma\right)\exp\left(\frac{-h_0\Gamma}{\tau_s}\right) \qquad (7b)$$

where h_0 is the initial hardening modulus, τ_o the initial yield shear stress, τ_s the saturation yield shear stress, h_1 the final hardening. Note that τ_s is defined in absolute terms and should be higher than τ_0. Finally, Γ is the accumulated shear strain in all slip systems as given by,

$$\Gamma=\int_0^t \sum_\alpha \dot{\gamma}_\alpha dt \qquad (8)$$

3. Time discretization

The non-linear global FE problem is linearized by applying the boundary conditions (loads or applied displacements) as a function of time and discretizing this time in increments Δt. The solution for each time increment is obtained iteratively using a Newton-Raphson approach. Each global iteration corresponds, at the integration point level, to a given prediction of the deformation gradient tensor, $F_{t+\Delta t}$.

Let *t* be the last converged time, then at each integration point the variables $F_t, F^e{}_t, F^p{}_t, \sigma_t$ are known as well as a set of internal variables α_t. The global solver

provides a prediction of $F_{t+\Delta t}$ and the constitutive equation has to determine these other magnitudes: $\sigma_{t+\Delta t}$, $\alpha_{t+\Delta t}$ and $\frac{\partial \Delta \sigma}{\partial \Delta \varepsilon}$

The crystal plasticity routine consists then in an implicit method to solve the equations (1-8) where the inputs and outputs are:

INPUTS: $F_t, F^e{}_t, F_{t+\Delta t}, \gamma^\alpha{}_t, \quad g^\alpha{}_t$

OUTPUTS : $\sigma_{t+\Delta t}$, $\frac{\partial \Delta \sigma}{\partial \Delta \varepsilon}$ and $, \gamma^\alpha{}_{t+\Delta t}, \quad g^\alpha{}_{t+\Delta t}$

The integration method developed is based on the exponential map operator [8] and the non-linear algebraic system (1-8) between t and t+Δt is solved by two Newton-Raphson schemes: Let $F^e{}_0$ be the elastic deformation gradient prediction for t+Δt,

$$F_{t+\Delta t} F_t^{-1}$$
¿ F^e
¿
$F^e{}_0 =$ ¿ (9)

Then the set of equations (3,4,5) provide the actual value of $F^e{}_{t+\Delta t}$ as the solution of the implicit equation (10)

$$F^e{}_{t+\Delta t} = F^e{}_0 \exp\left(-\Delta t \cdot \sum_\alpha \dot{\gamma}^\alpha \left(F^e{}_{t+\Delta t}, \alpha_{t+\Delta t}\right) s^\alpha \otimes m^\alpha\right) \quad (10)$$

An “external” Newton-Raphson scheme is developed that tries to solve equation (10), searching for the actual values of $F^e{}_{t+\Delta t}$ that solve equation (10). In addition, for each iteration of $F^e{}_{t+\Delta t}$ another Newton-Raphson scheme can be used for an implicit evolution of hardening (to obtain the values of $\alpha_{t+\Delta t}$), otherwise the evolution of $g^\alpha{}_{t+\Delta t}$ is done in an explicit manner.

4. Subroutine INPUTS

The model is implemented as a material subroutine (umat subroutine in ABAQUS). The material properties, orientation, etc are defined in two parts:

A) First, within the abaqus input file must include the name and orientation (Fig 1) of the material respect to a global system. This done using the

*MATERIAL,NAME=XXX
*USER MATERIAL, TYPE=MECHANICAL,CONSTANTS=7
v1x,v1y,v1z,v2x,v2y,v2z,thetax

Where v_1, v_2 correpond to vectors [100] and [001] expressed in the global system ($\mathbf{e_x}, \mathbf{e_y}, \mathbf{e_z}$),Fig 1. The last value, thetax, corresponds to an additional rotation around global x axis.

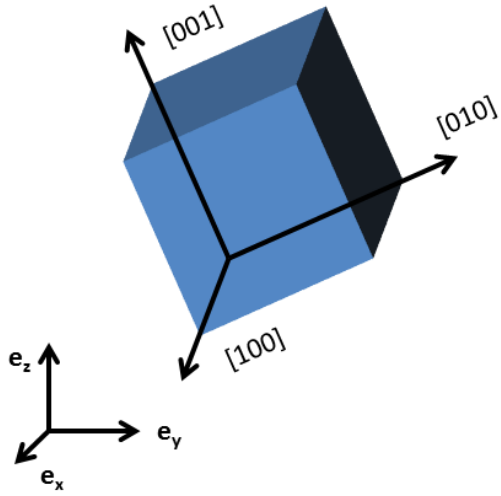

Figure 1: Orientation of single crystal respect to a global system

B) Second, an input file where the crystal properties are specified. The file is an ascii file, should be in the same directory as the inut file and the name is "crystal.prop". This file includes

- the elastic properties of the crystal ($C, eq.5¿.$ If general orthotropic C_{11}, C_{12} $C_{44,}$ C_{13},C_{33},$C_{66.}$.If orthotropic with equivalent axis C_{11}, C_{12} and $C_{44.}$ Subroutine determines symmetry with the number of given properties. C_{33} is used for directions 2 and 3, C_{66} corresponds to shear in 1-2, and C_{44} to shear in 1-3 and 2-3
- the parameters of the viscous power law ($\dot{\gamma}_0$ and *m*, eq. 4)
- The number of slip system sets N. In FCC normaly only one set is active ([111]<110>), but in HCP there exist the basal set, pyramidal, etc.... For each set

(A,B,...N) the file includes the definition of the slip systems by their tangent and normal vectors (s^{α} and m^{α} respectively for α=1,...n)

- The hardening coefficients between sets q_{AB} , for A=1,..N, B=1,..N
- The single crystal hardening parameters:
  - o if Asaro Needleman law (h_0 , $\tau_o \wedge ¿$ τ_s),eq (7a)
  - o If Voce h_0 , τ_o, τ_s and h_1 , eq (7b)
- Some internal parameters to control the newton-raphson iterations: TOLER,TOLER_jac,NITERMAX,NITERMAX_jac,strain_inc_jac,implicit_hard. The first two are NR tolerances for integrating the step (from $t \rightarrow t+\Delta t$) and for integrating a perturbation of the step in order to obtain the Jacobian matrix (from $t \rightarrow t+\Delta t+\delta t$). NITERMAX,NITERMAX_jac are the maximum number of iterations allowed for the integration of step and perturbated step respectively. strain_inc_jac is the size of the strain perturbations for the jacobian,and finally implicit_hard is a flag (1 or 0), that enables and disables the implicit calculation of hardening.

An example of a crystal.prop file for an FCC crystal based on an Al alloy is given below:

```
# Name: AA6116 Al
# C11, C12,C14
108d3,62d3,28d3
#Viscoplastic law: gamma_0, exponent
1.,0.1
# Set of slip systems, Total number of systems
1,12
# normalv, tangent, set
 1 , 1 , 1 , 1 , -1 , 0,   1
 1 , 1 , 1 , 0 , -1 , 1,   1
 1 , 1 , 1 , -1 , 0 , 1 ,   1
 1 , -1 , 1 , 1 , 1 , 0,   1
 1 , -1 , 1 , 0 , 1 , 1 ,   1
 1 , -1 , 1 , -1 , 0 , 1 ,   1
-1 ,-1 , 1 , 1 , -1 , 0 ,   1
-1 ,-1 , 1 , 0 , 1 ,  1 ,   1
-1 ,-1 , 1 , 1 , 0 ,  1 ,   1
 -1 ,1 , 1 , 1,  1 ,  0 ,   1
 -1 ,1 , 1 , 0 , -1 ,1 ,   1
 -1 ,1 , 1 , 1 , 0 , 1 ,   1
# q(alfa,alfa), q(alfa,beta)
```

```
1.
# Single crystal behavior based on Asaro-Needleman: tau0,taus,h0
116,119,793
# Control of subroutine:
NTOLER,NTOLER_jac,NITERMAX,NITERMAX_jac,strain_inc_jac,implicit_ha
rd
.5D-5,.5D-5,40,20,5D-5,1
```

5. OUTPUTS and state variables:

Several internal variables are defined and saved for calculation purposes and also for visualization (saved on the ODB file)

STATEV(1)-STATEV(9), 9 components of F^e_t

STATEV(9+1)-STATEV(9+NSYSTEMS), γ^α , α=1, NSYSTEMS

STATEV(9+1+NSYSTEMS)-STATEV(9+2*NSYSTEMS), g^α , α=1, NSYSTEMS

STATEV(10+2*NSYSTEMs)-STATEV(18+2*NSYSTEMS), 9 components of L^p_t

STATEV(19+2*NSYSTEMS)-(21+2*NSYSTEMS), the three euler angles respect to global axis (including both initial orientation and elastic rotations)

STATEV(22+2*NSYSTEMS), accumulated total plastic shear Γ

Examples, for a standard FCC it exist one set and 12 systems so number of STATEVS is 22+2*12=46 and in a HCP with 24 systems STATES is 22+2*24=70

6. Final considerations

In its actual form, the user subroutine solves the non-linear equations to obtain $\sigma_{t+\Delta t}$ using Newton-Raphson and analytical derivation of the residuals. On the contrary, the tangent stiffness matrix (DDSDDE in ABAQUS UMAT) is obtained numerically by performing perturbations of $F_{t+\Delta t}$ after achieving the equilibrium, see work of Kalidindi et al. in 1991 [9]

Subroutine works fine under abaqus v.6.7 and later with fortran v10 and later. The subroutine can be also run in parallel calculations but care must be taken when writing data to log file.

7. Examples

Attached to the document 6 files are given

SUBROUTINE:

umat_crysplas_ABQ_v5.f subroutine source code

subroutine_v4.f auxiliar subroutines

ABAQUS INPUT FILES:

1element_111.inp Example with 1 element: Uniaxial tensile deformation of 100% in 111 direction

2elements_111.inp Example of a bi-crystal made of 2 elements and same loading conditions than former example

EXAMPLE OF PROPERTY FILES:

crystal_FCC.prop Crystal properties of Al (FCC)

crystal_Mg.prop Crystal properties of Mg (HCP) without twinning

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