3.12 Material Model Type: *cp*

Crystal plasticity (CP) models simulate micro-scale deformation of metal alloys. CP models average the inherently discrete processes that drive metal plasticity (dislocation transport) into a continuum theory of deformation, suitable for finite element simulations. The CP model best represents deformation on the scale of several grains (polycrystal deformation), though it may also realistically represent large single crystals.

Crystal plasticity models differ from typical continuum material models employed in finite element analyses in that two distinct types of parameters define the material properties. The first type includes the usual values for elastic constants, flow properties, thermal expansion coefficients, etc. The second type include a set of Euler angles and the initial orientation of the atomic (crystal) lattice relative to some reference configuration. In most situations, a finite element model will adopt one set of material parameters but many different crystal orientations. In contrast for an alloy with multiple phases, materials may be defined with combinations of multiple sets of crystal parameters and lattice orientations.

Depending on the intended length-scale of the finite element simulation, each element may have: (1) a single crystal orientation and a single set of material properties or (2) many crystal orientations (polycrystal homogenization). *Both options are available in WARP3D.* To facilitate input, the CP material model separates the definitions of crystal (elastic and flow) properties, orientations, possible combinations of crystal properties, orientations, and other miscellaneous physical properties such as mass density and thermal expansion coefficient.

Appendix K provides a more comprehensive description of the CP model formulation.

3.12.1 Formulation

Kinematic Assumptions

The CP model in WARP3D closely follows the formulation presented in [1]. Unfortunately, CP models must distinguish elastic and plastic rotations, which makes them unsuitable for hypoelastic formulations. We present the model as hyperelastic; WARP3D handles the additional calculations and rotations required to bring the true Cauchy stresses the CP model calculates into the hypoelastic *unrotated* frame (similar to how WARP3D handles hyperelastic UMATs, see Section 3.11).

The CP model takes as input the deformation gradient $\mathbf{F}_{n+1}$ and the temperature T_{n+1} and returns the updated Cauchy stress $\boldsymbol{\sigma}_{n+1}$ – while maintaining a set of internal history variables. The stress update is based on the kinematic assumptions:

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p \tag{3.12.1}$$

$$\mathbf{F}^e = (\mathbf{I} + \boldsymbol{\varepsilon})\, \mathbf{R}^e \quad \boldsymbol{\varepsilon} \ll \mathbf{I} \tag{3.12.2}$$

$$\bar{\mathbf{L}}^p = \sum_{i=1}^{n} \dot{\gamma}^{(s)} \left(\bar{\mathbf{b}}^{(s)} \otimes \bar{\mathbf{n}}^{(s)} \right) \tag{3.12.3}$$

where $\bar{\mathbf{L}}^p = \dot{\mathbf{F}}^p \mathbf{F}^{p-1}$, $\bar{\mathbf{b}}^{(s)}$ is the slip direction vector of system s, $\bar{\mathbf{n}}^{(s)}$ is the slip plane normal vector of system s and $\dot{\gamma}^{(s)}$ is given by:

$$\dot{\gamma}^{(s)} = \frac{\dot{\gamma}_0}{\tilde{\tau}} \left| \frac{\tau^{(s)}}{\tilde{\tau}} \right|^{n-1} \tau^{(s)} \tag{3.12.4}$$

with $\tau^{(s)}$ the resolved shear on system s ($\tau^{(s)} = \left[\mathbf{R}^e \mathbf{m}_s^{(s)} \left(\mathbf{R}^e\right)^T\right] : \boldsymbol{\tau}$, with $\boldsymbol{\tau}$ the Kirchhoff stress and $\mathbf{m}_s^{(s)} = \left(\bar{\mathbf{b}}_s^{(s)} \otimes \bar{\mathbf{n}}_s^{(s)}\right)_{\text{sym}}$), $\dot{\gamma}_0$ some reference strain rate, taken to be $\dot{\gamma}_0 = \sqrt{\frac{2}{3}\mathbf{D} : \mathbf{D}}$, with $\mathbf{D}$ the symmetric part of the spatial velocity gradient, and $\tilde{\tau}$ some slip system strength, defined in the section on work-hardening below. Equation 3.12.1 is common to nearly all current theories of plastic deformation. Plastic deformation of metals generally results in small elastic stretch (but possibly large elastic rotation), which justifies Eq. 3.12.2. The decomposition of polyslip into a series of simple shear deformations justifies Eq. 3.12.3. Equation 3.12.4 derives from empirical observation of material response..

We assume $\mathbf{R}^e$ (the elastic rotation): (1) varies slowly in time, (2) remains fixed over a time (load) step and (3) updates with an explicit integration. We integrate a stress-rate equation implicitly to find the Kirchhoff stress $\boldsymbol{\tau}^{n+1}$. Following a lengthy derivation, the result becomes a nonlinear system of equations to compute the updated stress at $n+1$:

$$\begin{aligned}
\boldsymbol{\tau}_{n+1} &= \boldsymbol{\tau}_n + \Delta t \mathbf{C}_n^* \left(\mathbf{D}_{n+1} - \hat{\mathbf{D}}_{n+1}^p + \mathbf{S}_n^* \boldsymbol{\tau}_{n+1} \hat{\mathbf{W}}_{n+1}^p - \hat{\mathbf{W}}_{n+1}^p \mathbf{S}_n^* \boldsymbol{\tau}_{n+1} \right) \qquad (3.12.5) \\
\hat{\mathbf{D}}_{n+1}^p &= \sum_{s=1}^{N} \dot{\gamma}_{n+1}^{(s)} \left[\mathbf{R}_n^e \mathbf{m}_s^{(s)} \left(\mathbf{R}_n^e\right)^T \right] \\
\hat{\mathbf{W}}_{n+1}^p &= \dot{\mathbf{R}}_n^e \left(\mathbf{R}_n^e\right)^T + \sum_{s=1}^{N} \dot{\gamma}_{n+1}^{(s)} \left[\mathbf{R}_n^e \mathbf{q}_s^{(s)} \left(\mathbf{R}_n^e\right)^T \right]
\end{aligned}$$

with $\mathbf{q}_s^{(s)} = \left(\bar{\mathbf{b}}_s^{(s)} \otimes \bar{\mathbf{n}}_s^{(s)}\right)_{\text{anti}}$. The Cauchy stress is then simply $\boldsymbol{\sigma}_{n+1} = \boldsymbol{\tau}_{n+1}/J_{n+1}$with $J_{n+1} = \det \mathbf{F}_{n+1}$. The material model routines solve this equations with Newton's method. After a successful stress update, the CP model updates the elastic rotation with the explicit, Euler exponential integration:

$$\begin{aligned}
\mathbf{R}_{n+1}^* &= \exp \left\{ \left[\mathbf{W}_{n+1} - \sum_{s=1}^{N} \dot{\gamma}_{n+1}^{(s)} \left[\mathbf{R}_n^e \mathbf{q}_s^{(s)} \left(\mathbf{R}_n^e\right)^T \right] - \right. \qquad (3.12.6) \\
&\qquad \left. \left(\boldsymbol{\varepsilon}_{n+1} \hat{\mathbf{D}}_{n+1}^p - \hat{\mathbf{D}}_{n+1}^p \boldsymbol{\varepsilon}_{n+1} \right) - \frac{1}{2} \left(\boldsymbol{\varepsilon}_{n+1} \dot{\boldsymbol{\varepsilon}}_{n+1} - \dot{\boldsymbol{\varepsilon}}_{n+1} \boldsymbol{\varepsilon}_{n+1} \right) \right] \Delta t \right\} \mathbf{R}_n^e
\end{aligned}$$

This description of the model here necessarily omits many details of the derivation (see Appendix K for a more complete discussion).

In addition to updated stresses at $n+1$, the material model routines must return the consistent tangent modulus for use in the global Newton iterations (again, we omit the derivation).

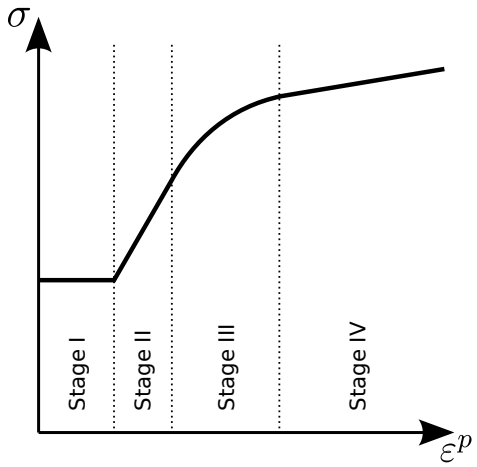

Figure 3.12.1: Stages of work hardening. Most metal alloys do not exhibit Stage I behavior.

The flow rule of Eq. 3.12.3 is non-associative which leads to a non-symmetric consistent tangent matrix. WARP3D and its solvers currently process only symmetric systems of equations. The CP model computes an approximate, symmetrized tangent. Since this is only an approximate tangent, the global Newton iterations may not achieve true quadratic convergence. Users should expect the potential of additional Newton iterations per load step, and generally must specify smaller increments of load per step to achieve good convergence rates.

Work Hardening

We have not yet defined the slip system strength $\tilde{\tau}$. This value represents both the initial strength of the system from inherent obstacles to dislocation motion (the *yield stress*), and the increase in strength due to forest dislocation hardening (*work hardening*). The total strength is thus:

$$\tilde{\tau} = \tau_a + \tau_y\left(T, \dot{\varepsilon}\right)\frac{\mu}{\mu_0} + \bar{\tau}\left(\varepsilon_p, T, \dot{\varepsilon}\right)\frac{\mu}{\mu_0} \tag{3.12.7}$$

which explicitly separates temperature and rate invariant components of the yield stress (τ_a) from those dependent on temperature and rate (τ_y). The work hardening component ($\bar{\tau}$) might depend on both rate and temperature in addition to the amount of accumulated plastic strain. The μ/μ_o ratio accounts for temperature dependent elastic properties.

Work hardening behavior follows the stages illustrated in Fig. 3.12.1. The infrequent Stage I behavior characteristic of Luders bands is not considered here with efforts focused on Stages II, III, and IV. Stage II has a constant slope ($d\sigma/d\varepsilon^p$), Stage IV has a small constant slope, and Stage III transitions between the two. A linear Voce Law shown in Fig. 3.12.2 defines the Stage III transition. For the moment, let the final, Stage IV slope be zero. Then the Voce Law becomes:

$$\frac{d\bar{\tau}}{dt} = \sum \theta_0 \left\{1 - \frac{\bar{\tau}}{\tau_v\left(T, \dot{\varepsilon}\right)}\right\}\left|\dot{\gamma}^{(s)}\right| \tag{3.12.8}$$

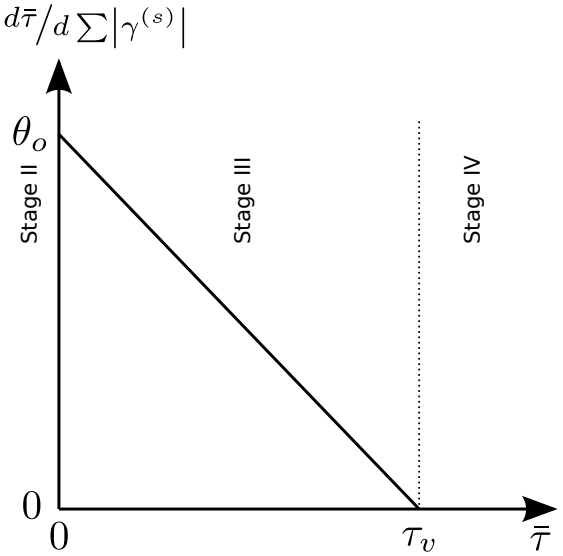

Figure 3.12.2: Simplified Voce Law evolution of work-hardening slope. Here Stage II is the instantaneous starting slope θ_0 and the final Stage IV slope is 0.

where we replace $d\sigma$ with $d\bar{\tau}$ and $d\varepsilon^p$ with $\left|\dot{\gamma}^{(s)}\right| dt$. We can view $\tau_v\left(T,\dot{\varepsilon}\right)$ as the saturation strength of work hardening for a given temperature and rate. The parameter θ_0 determines the initial Stage II hardening slope. Determining the slip system strength then reduces to choosing functional forms for $\tau_y\left(T,\dot{\varepsilon}\right)$ and $\tau_v\left(T,\dot{\varepsilon}\right)$ and integrating the Voce Law.

The Mechanical Threshold Strength Kocks, Argon, and Ashby developed one theory for $\tau_y\left(T,\dot{\varepsilon}\right)$ and $\tau_v\left(T,\dot{\varepsilon}\right)$ called the Mechanical Threshold Stress (MTS, [2]). Simply put, the MTS is the value τ_y or τ_v would have with no thermal or rate activation energy, that is $\tau\left(0,0\right)$. Define this value to be $\hat{\tau}$ (the MTS). Kocks, Argon, and Ashby proposed an Arrhenius-type scaling law to bring this MTS to a given combination of rate and temperature:

$$\tau = \hat{\tau}\left[1-\left(\frac{kT}{\mu\left(T\right)b^3 g_0^{(i)}}\ln\frac{\dot{\varepsilon}_0^{(i)}}{\dot{\varepsilon}}\right)^{\frac{1}{q^{(i)}}}\right]^{\frac{1}{p^{(i)}}} \tag{3.12.9}$$

where k is the Boltzmann constant, T is absolute temperature, b is the magnitude of the Burger's vector, $g_0^{(i)}$ is a normalized activation energy, $\dot{\varepsilon}_0^{(i)}$ is a reference strain rate, and $q^{(i)}$ and $p^{(i)}$ are constants related to the shape of the activation energy barrier. Applying this concept to the work hardening model (Eqs. 3.12.7 and 3.12.8) we have:

$$\tau_y\left(T,\dot{\varepsilon}\right) = \hat{\tau}_y\left[1-\left(\frac{kT}{\mu\left(T\right)b^3 g_{0,y}}\ln\frac{\dot{\varepsilon}_{0,y}^{(i)}}{\dot{\gamma}_0}\right)^{\frac{1}{q_y}}\right]^{\frac{1}{p_y}} \tag{3.12.10}$$

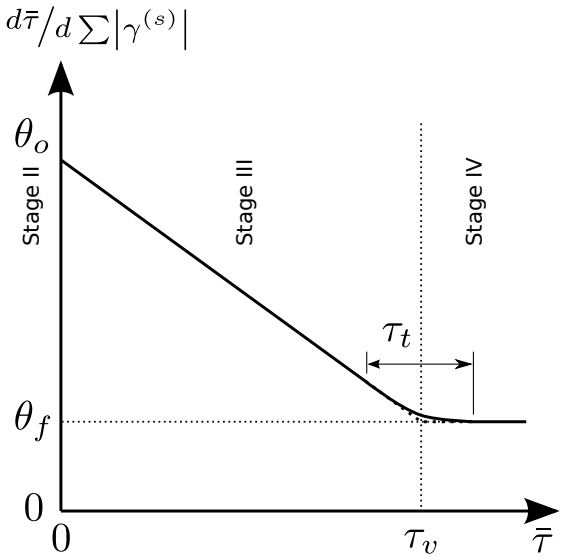

Figure 3.12.3: Voce law modified for empirical Stage IV hardening. θ_f and τ_t are new parameters.

$$\tau_v\left(T,\dot{\varepsilon}\right)=\hat{\tau}_v\left[1-\left(\frac{kT}{\mu\left(T\right)b^3g_{0,v}}\ln\frac{\dot{\varepsilon}_{0,v}^{(i)}}{\dot{\gamma}_0}\right)^{\frac{1}{q_v}}\right]^{\frac{1}{p_v}} \tag{3.12.11}$$

In these equations the $\hat{\tau}$, g_0, $\dot{\varepsilon}_0$, q, and p terms are parameters, b and k are physical constants, and we adopt the form:

$$\mu\left(T\right)=\mu_0-\frac{D_0}{\exp\left(T_0/T\right)-1} \tag{3.12.12}$$

for the temperature-dependent shear modulus, where μ_0, D_0, and T_0 are all parameters. The CP model in WARP3D implements this hardening formulation with an implicit integration of Eq. 3.12.7. This introduces an additional equation into the local (material) nonlinear system of Eq. 3.12.5, which in turn expands its linearization in Newton's method by one row and column.

Stage IV Hardening

The CP model provides two approaches to Stage IV hardening. The first adopts a constant, terminal Stage IV hardening slope, much like the model specifies the Stage II slope in Eq. 3.12.8. In addition, to avoid a sharp transition in slope between Stage III and Stage IV, we smooth the transition with a cubic spline (see Fig. 3.12.3). This requires some modification to Eq. 3.12.8 and introduces the parameters θ_f (the terminal Stage IV slope) and τ_t (the width of the transition region). This simple model is integrated implicitly.

A second approach includes the effect of Geometrically Necessary Dislocations (GNDs). GNDs are those (theoretically) necessary to maintain compatible deformation (for early work

see [3]). Researchers argue these necessary dislocations are distinct from the statically stored dislocations associated with forest hardening, and therefore contribute to a different hardening mechanism. Acharya *et al.* associate these geometric dislocations with Stage IV hardening [4]. Omitting some derivation and theory (see references for details), the Nye's tensor of geometrically necessary dislocations is:

$$\boldsymbol{\alpha} = -\nabla \times \mathbf{F}^{e-1}$$

The density of necessary dislocations along each slip system is:

$$\lambda^{(s)} = \sqrt{\left(\boldsymbol{\alpha}\mathbf{n}_s^{(s)}\right) : \left(\boldsymbol{\alpha}\mathbf{n}_s^{(s)}\right)}$$

Archarya *et al.* show a reasonable addition to the Voce law, accounting for GNDs is:

$$\frac{d\bar{\tau}}{dt} = \sum \theta_0 \left\{ 1 - \frac{\bar{\tau}}{\tau_v} + \frac{\tau_\lambda^{(s)}}{\bar{\tau}} \right\} \left| \dot{\gamma}^{(s)} \right| \tag{3.12.13}$$

$$\tau_\lambda^{(s)} = \frac{k_0}{k_1} \eta\mu\lambda^{(s)} \tag{3.12.14}$$

In Eq. 3.12.14 $k_1 = 2\theta_0 / \left(\eta\mu\left(T\right) b\right)$, $\eta = 1/3$, and k_0 is a parameter (reasonable values are on the order of 1). Calculating the curl of the elastic deformation through an implicit integration is very difficult; consequently, we update the values of $\tau_\lambda^{(s)}$ explicitly. The remainder of the hardening evolution remains implicit, as above.

Polycrystal Homogenization

Some computational models represent each grain in a polycrystal aggregate using multiple finite elements. Such models enforce compatibility of deformation via shared nodal displacements and displacement compatible element formulations. Stress equilibrium is enforced weakly through the Galerkin weak form.

In other computational models, techniques are employed that group many crystals into a single polycrystal – often at an integration point in a finite element model. These are termed polycrystal homogenization methods; they represent a natural approach to create reduced, multi-scale models. With an appropriate homogenization technique, single finite elements on the scale of centimeters can represent an aggregated microstructure of grains with a length-scale on the order of microns.

The CP model in WARP3D provides Taylor-homogenized (constant-deformation/strain) polycrystals, where each finite element represents multiple crystals. With the Taylor approximation, the strain (rate of strain) in each grain remains fixed at the global value, and the resulting (not necessarily equilibrium) stresses are averaged.

3.12.2 Crystal Definition

A *crystal* defines a set of elastic, flow, and hardening properties. Commonly, each phase in the material will be a different crystal. Crystals are defined in the analysis input file and assigned a number by the user. Crystal numbers must start at 1 and increase sequentially. The following shows an example crystal definition:

```
crystal 1
      properties slip_type fcc elastic_type isotropic,
      e 78811.2 nu 0.33,
      mu_0 29628.3 D_0 0.0 t_0 204.0 harden_n 20,
      theta_0 180.0,
      b 3.5E-7 boltz 1.3806E-20,
      tau_a 0.0,
      tau_hat_y 155.0 g_0_y 0.007808 q_y 2.0 p_y 0.5,
      eps_dot_0_y 1.0E13,
      tau_hat_v 25.0 g_0_v 0.00488 q_v 2.0 p_v 0.5,
      eps_dot_0_v 1.0E7,
      hardening geometric k_0 5.0
```

Tables 3.1, 3.2, 3.3, and 3.4 detail all parameters for crystal definitions. Note that elastic properties of the material are temperature invariant at this time, while the plastic properties vary with temperature. Since the shear modulus of the material is both a plastic material property and an elastic property, it must be defined twice for cubic, elastic anisotropy.

The keywords `mu_0`, `D_0`, and `t_0` set properties in Eq. 3.12.12 above to define the temperature-dependent shear modulus for the plastic hardening equations.

If the material is isotropically elastic, do not set a value for the shear modulus.

For cubic anisotropy, users must enter a second (constant) value for the shear modulus using the keyword `mu`. This second value is only for the purpose of defining the constant elasticity tensor.

If the shear modulus in the hardening equations and in the elasticity tensor both should be constant, set `mu_0` to the constant value and set `D_0` $= 0$.

The definition of the remaining properties should be clear with reference to the noted equations and the previous section on the model formulation. The model implementation is not restricted to FCC, BCC, and HCP systems. Research users of WARP3D can add additional slip system types by altering the source file mod_crystals.f. Similarly, users could add additional constant elasticity tensors by altering the same file.

3.12.3 Material Definition

A complete *material* definition to set properties of finite elements in WARP3D for the CP model requires: (1) at least one crystal, (2) crystal orientation, and (3) some miscellaneous properties. Users can provide crystals (see 3.12.2) and orientation Euler angles through two mechanisms – either directly in the definition of the material in the analysis input file or using a separate (flat) text file.

These parameters can be specified using combinations of both mechanisms as proves most conventient: (1) direct specification of the crystal number, with a file for the angle specifications,

Property	Keyword	Options/type
Slip system type	slip_type	fcc, bcc, hcp
Elastic type	elastic_type	isotropic, cubic
Young's modulus	e	real
Poisson's ratio	nu	real
Shear modulus (elastic)	mu	real
μ_0 (Eq. 3.12.12)	mu_0	real
T_0 (Eq. 3.12.12)	T_0	real
D_0 (Eq. 3.12.12)	D_0	real
Boltzmann constant	k	real
Magnitude of Burgers vector	b	real
n (Eq. 3.12.4)	harden_n	real
τ_a (Eq. 3.12.7)	tau_a	real

Table 3.1: General crystal properties.

Property	Keyword	Options/type
$\hat{\tau}_y$	tau_hat_y	real
$g_{0,y}$	g_0_y	real
q_y	q_y	real
p_y	p_y	real
$\dot{\varepsilon}_{0,y}$	eps_dot_0_y	real

Table 3.2: Properties related to τ_y, refer to Eq. 3.12.10 above.

(2) vice versa, and (3) direct specification of both the crystal number and the Euler angles, or (4) a separate file for both.

The main drawback to direct specification of one set of parameters in the material definition is that only a single crystal or orientation can be entered – using this option for both the crystal number and orientation precludes the definition of a homogenized polycrystal. In addition, in a model with many grains (regions of different orientations) assigning each grain its own material model will quickly become cumbersome. Defining orientations (and/or crystal types) through a separate file avoids both difficulties and is the recommended approach.

The keyword `crystal_input` determines how the material specifies the crystal numbers. If

Property	Keyword	Options/type
$\hat{\tau}_v$	tau_hat_v	real
$g_{0,v}$	g_0_v	real
q_v	q_v	real
p_v	p_v	real
$\dot{\varepsilon}_{0,v}$	eps_dot_0_v	real
θ_0	theta_0	real

Table 3.3: Properties related to τ_v, refer to Eq. 3.12.11 above.

Property	Keyword	Options/type
Stage IV hardening type	hardening	empirical, geometric
θ_f (Fig. 3.12.3)	theta_f	real
τ_t (Fig. 3.12.3)	tau_t	real
k_0 (Eq. 3.12.14)	k_0	real

Table 3.4: Properties related to Stage IV hardening.

`crystal_input` is set to `single`, then the command must be followed by `crystal_type <int>`, where `<int>` is an integer corresponding to a valid crystal number.

If `crystal_input` is set to `file`, then the command must be followed by `filename <string>` where `<string>` is the filename of a flat ASCII file with format described in the next paragraph.

The keyword `angle_input` similarly defines how the orientation(s) for the material model are input. If `angle_input` is followed by `single` then the command `angles <float> <float> <float>` must subsequently appear in the material definition, where the three floats are the Euler angles defining the material's crystallographic orientation. If `angle_input` is followed by `file` then `filename <string>` must be a flat file, with format defined below. Currently, Euler angles must use the symmetric Kocks convention. The model uses this convention internally.

The file referenced by the `filename` command should be a (flat) ASCII file with one or more records for each finite element using the material, one record per line, with records generated using the format:

$$< \text{int} > < \text{int} > < \text{float} > < \text{float} > < \text{float} >$$

The first integer is the finite element number. The second integer is the crystal number for this element. This part of the record is present only if the `crystal_input file` specification was used. The next three floating point numbers are the Euler angles for this element. This part of the record is present only if the option `angle_input file` is used.

Each element can have more than one entry – in which case the material model assumes the element represents a Taylor-homogenized polycrystal. Conditions on the element entries: (1) the number of entries per element must correspond to the parameter `n_crystals` (*i.e.* each element number must appear `n_crystals` times) and (2) elements must appear in sequential, numerical order (all crystals in the first element using the material, then all crystals in the second element, and so on in numerical order).

Table 3.5 describes the remaining material options. The `tolerance` parameter refers to the local, material (Newton) iterations to compute the new converged stress state. The `debug` option turns on a variety of print statements inside the CP computation routines.

3.12.4 Model Output

The model provides the usual stresses, strains, and energy densities for output. It currently outputs a single material model state variable into *mat_val1*, the Mises equivalent plastic strain, from the integral:

$$\bar{\varepsilon}^p = \int \sqrt{\frac{2}{3}\mathbf{D}^p : \mathbf{D}^p}\, dt \tag{3.12.15}$$

Property	Keyword	Options/type
Euler angle convention	angle_convention	kocks
Isotropic thermal expansion coefficient	alpha	real
Mass density	rho	real
Local convergence tolerance	tolerance	real
Number of crystals per material point	n_crystals	integer
Euler angle type	angle_type	degrees, radians
Crystal input type	crystal_input	single, file
Crystal number (if single input)	crystal_type	integer
Euler angle input type	orientation_input	single, file
Euler angles (if single input)	angles	real, real, real
Name of input file (if file input)	filename	string
Debug flag	debug	on, off

Table 3.5: Material model properties and options.

In addition to this material state variable, the CP model introduces an entirely new Patran element result file (see Section 2.12 for an overview on Patran compatible result files). This result file can be requested with the WARP3D output command:

$$\underline{\text{output}}\ \underline{\text{patran}} \left\{ \begin{array}{c} \underline{\text{binary}} \\ \underline{\text{formatted}} \end{array} \right\} \underline{\text{element}}\ \underline{\text{states}}$$

The element state files have filenames *we(b/f)m######*where *(b/f)* is *b* if binary files are requested or *f* if formatted files are requested and ###### is the step number. The *patran_templates* directory in the WARP3D distribution contains a file (*warp_elem_mm10.res_tmpl*) which has natural language descriptions of each column of output in the *webm* and *wefm* files. The variables output are listed in Table 3.6.

The file contains one record for each finite element assigned a CP material. Computed values are those averaged over all integration points of the element.

Quantity	Description	Number of columns
nslip	Number of slip systems	1
tau_bar	Work hardening strength $\bar{\tau}$	1
tau_v	Saturation strength τ_v	1
slip	Total accumulated slip on systems 1-24	24
Fe	Components of $\mathbf{F}^e$	9
curl-Fe	Components of $\nabla \times \mathbf{F}^{e-1}$	9
e-stretch	Components of ε (Voigt notation)	6
e-rot	Components of $\mathbf{R}^e$	9
euler	Updated Euler angles, in Kocks convention	3

Table 3.6: Variables output in Patran style *element state file.*

3.12.5 Examples

Crystal Definition – Isotropic Elasticity and Empirical Stage IV Hardening

This crystal is isotropically elastic, with a constant value of μ for the hardening equations. This example employs the empirical Stage IV hardening option.

Note that all values are defined on a single, logical line of input continued across multiple physical lines with commas.

Physical units for all examples are MPa, mm, N, and mJ.

```
crystal 1
      properties slip_type fcc elastic_type isotropic,
      e 70000.0 nu 0.30,
      mu_0 26923.1 D_0 0.0 T_0 204.0 harden_n 20,
      theta_0 2000.0,
      b 3.5E-7 boltz 1.3806E-20,
      tau_a 5.0,
      tau_hat_y 155.0 g_0_y 0.007808 q_y 2.0 p_y 0.5,
      eps_dot_0_y 1.0E13,
      tau_hat_v 25.0 g_0_v 0.00488 q_v 2.0 p_v 0.5,
      eps_dot_0_v 1.0E7,
      hardening empirical theta_f 200.0 tau_t 30.0
```

Crystal Definition – Anisotropic Elasticity and Geometric Hardening

This crystal definition demonstrates the options for cubic elastic anisotropy, temperature dependent shear modulus, and geometric hardening.

```
crystal 2
      properties slip_type bcc elastic_type cubic,
      e 70000.0 nu 0.30 mu 37000.0,
      mu_0 37000.0 D_0 1000.0 T_0 204.0 harden_n 20,
      theta_0 2000.0,
      b 3.5E-7 boltz 1.3806E-20,
      tau_a 5.0,
      tau_hat_y 155.0 g_0_y 0.007808 q_y 2.0 p_y 0.5,
      eps_dot_0_y 1.0E13,
      tau_hat_v 25.0 g_0_v 0.00488 q_v 2.0 p_v 0.5,
      eps_dot_0_v 1.0E7,
      hardening geometric k_0 1.0
```

Single Crystal Material – Properties in Material Definition

This example defines a simple, single crystal material with a single orientation. The material is defined completely inside the WARP3D input file – it does not refer to an external flat file.

```
material simple_cp
      properties cp alpha 1.08E-5 rho 0.0 angle_convention kocks,
      n_crystals 1 angle_type degrees,
      crystal_input single crystal_type 1,
      orientation_input single angles -108.11 45.3 17.2,
      debug off tolerance 1.0E-10
```

Single Crystal Material – Orientations in File

This material demonstrates the more common case – simulation of a single phase material, with each grain represented by many elements and many grains in the simulation model. A separate data file provides the material orientation for each finite element.

```
material simple_cp
      properties cp alpha 1.08E-5 rho 0.0 angle_convention kocks,
      n_crystals 1 angle_type degrees,
      crystal_input single crystal_type 1,
      orientation_input file filename 'angle_input',
      debug off tolerance 1.0E-10
```

Contes of the file `angle_input`:

```
      1        -37.63606 47.07174 53.69239
      2        -37.63606 47.07174 53.69239
      3        -37.63606 47.07174 53.69239
      4        -37.63606 47.07174 53.69239
      5        -45.11568 19.94000 9.48913
      6        -45.11568 19.94000 9.48913
      7        -45.11568 19.94000 9.48913
      8        -45.11568 19.94000 9.48913
      9        51.94430 30.14746 82.73049
      10       51.94430 30.14746 82.73049
      11       51.94430 30.14746 82.73049
      12       51.94430 30.14746 82.73049
      .
      .
      .
```

Here each grain is discretized with only four elements.

Polycrystal Material

This example uses a flat file to specify both the crystal number and the orientation for a six crystal, Taylor homogenized polycrystal.

```
material simple_cp
      properties cp alpha 1.08E-5 rho 0.0 angle_convention kocks,
      n_crystals 6 angle_type degrees,
      crystal_input file,
      orientation_input file filename 'angle_input',
      debug off tolerance 1.0E-10
```

And the flat file:

```
      1        1        -37.63606 47.07174 53.69239
      1        2        -42.17084 18.08290 45.31991
      1        1        137.61596 52.41387 45.10806
```

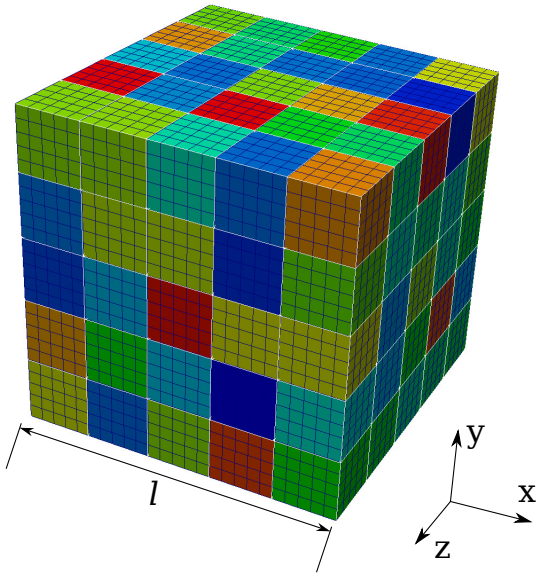

Figure 3.12.4: Example problem test_74.

```
1        2        110.92660 31.62225 52.36629
1        1        -45.11568 19.94000 9.48913
1        2        -64.65921 36.80016 78.43154
2        1        143.02645 45.44031 55.51358
2        2        66.58257 15.24942 79.21969
2        1        51.94430 30.14746 82.73049
2        2        -57.14742 24.13026 28.04172
2        1        -65.42632 45.87315 54.27781
2        2        73.70291 44.81913 35.88700
.
.
.
```

Test Problem Included in Distribution

The example problem shown in Fig. 3.12.4 is included in the WARP3D *verification* directory in the sub-directory *test74*. The simulation models a cube composed of $5 \times 5 \times 5$ cubic grains, each grain with its own orientation and discretized with $5 \times 5 \times 5$ elements. The assembled elements are loaded in uniaxial tension. All the grains have the same crystal definition and orientations are read from the file 'angle_input'.

3.12.6 References

[1] S. Kok, A. J. Beaudoin, and D. A. Tortorelli. A polycrystal plasticity model based on the mechanical threshold. *International Journal of Plasticity*, 18:715-741, 2002.

[2] U. F. Kocks, A. S. Argon, and M. F. Ashby. Thermodyanmics and kinetics of slip. In B. Chalmers, J. W. Christian, and T. B. Massalki, editors, *Progress in Materials Science*, vol. 19. Pergamon Press, 1975.

[3] M. F. Ashby. The deformation of plastically non-homogeneous materials. *Philosophical Magazine*, 21:399-424, 1970.

[4] A. Acharya, J. L. Bassani, and A. Beaudoin. Geometrically necessary dislocations, hardening, and a simple gradient theory of crystal plasticity. *Scipta Materialia*, 48:167-172, 2003.