# 49 Vgrain Abaqus Model

## Model information

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| Average grain diameter | 30 um |
| Size of 49grain model | 210\*210\*20\* um^3 |
| No. of grains | 49 |
| Type of deformation | yy Compression (top surface) |
| Total strain | 0.05 |
| Strain rate | 0.01 s^-1 |
| Boundary conditions | bot, 2, 2; right, 1, 1; back, 3, 3 top, 2, 2, -10.5 |
|  |  |
| Size of 4grain model | 60\*60\*20\* um^3 |
| No. of 4grain calibration grains | 4 |

## CPFE Model

The CPFE model has been demonstrated to capture single and multiple slip system activation and the full-filed heterogeneous strain distributions [14]. The model will be used in this project is rate-sensitive and implemented in the user material subroutine UMAT using ABAQUS standard/explicit analysis [15].

The total deformation gradient, , consists of elastic deformation gradient, , and plastic deformation gradient, , as . The elastic deformation gradient contributes to lattice rotation and stretch while the plastic deformation gradient contributes to slip and continuum rotation. The plastic velocity gradient, , is given by

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|  |  | **Equation 1** |

where  is the line vector along slip direction and  is the slip plane normal of slip system . The slip rate, , on the slip system  is given by

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|  |  | **Equation 2** |

where  is the mobile dislocation density,  is the magnitude of Burger’s vector,  is the jump frequency for driving thermally activated dislocation escape,  is the activation energy,  is the associated activation volume,  is the resolved shear stress and  is the critical resolved shear stress of the slip system . Hence, the accumulated slip on the slip system , , after a certain period,  is expressed as

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|  |  | **Equation 3** |

For modelling the plastic behaviour, a modified Taylor hardening rule used to describe the isotropic hardening is given by

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|  |  | **Equation 4** |

where  is the initial slip strength,  is the shear modulus,  is the geometrically dislocation density and  is the statistically stored energy. The evolution of SSD density has liner relationship with accumulated slip rate as

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|  |  | **Equation 5** |

where  is the hardening coefficient, and the effective plastic strain rate, , is expressed by

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|  |  | **Equation 6** |

The appearance of SSDs and GNDs induces the shear resistance on each slip system [14]. The GNDs are extra storage of dislocations to accommodate the lattice curvature where a non-uniform plastic deformation occurs [16]. Nye’s dislocation tensor using to compute the components of GNDs is given by

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|  |  | **Equation 7** |

where  are the screw dislocation components on slip system  with line vector along the slip direction ,  and  are the edge dislocation components with line tangent vector along the slip normal  and  respectively,  and  is the Burgers vector on slip system .

The 36 independent GND components, that include 12  crew, 12  edge and 12  edge dislocation components, need to be solved from the equations listed above. Equation 7 may be written in a matrix as

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|  |  | **Equation 8** |

where  is 91 vector form of the Nye’s dislocation tensor ,  is a 936 linear matrix containing the basis tensors ,  and  [17]. The sum of squares of GND densities on each slip is expressed as:

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|  |  | **Equation 9** |

The initial crystal slip strength  and isotropic hardening coefficient  in equations 4 and 2 were determined by matching the simulation results of polycrystalline metal response under tensile test with the experimental results [14]. The other material properties, such as the anisotropic elastic stiffness (i.e. Young’s modulus), Burger’s vector magnitude , Boltzman constant , initial mobile dislocation density  can be obtained from literature [14]. The activation energy  can be selected to give negligible rate sensitivity at room temperature.

## Material properties

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| Name | **My CPFE parameter** | **T. Takaki CPFE parameter (2007)** |
|  |  | 0.03 |
| Young’s modulus (E) | MPa | MPa |
| Shear modulus (G12) | 25.926 MPa | 25.926 MPa |
| Burger’s vector (b) | 2.86 um | 2.86 |
| Numerical vector | (u) 0.22 | (a) 0.1 |
| Poisson’s ratio | 0.35 | 0.345 |
| Gammast () | 0.1 |  |