PRISMS-Plasticity

Crystal Plasticity

Simple Tension Example -BCC Titanium

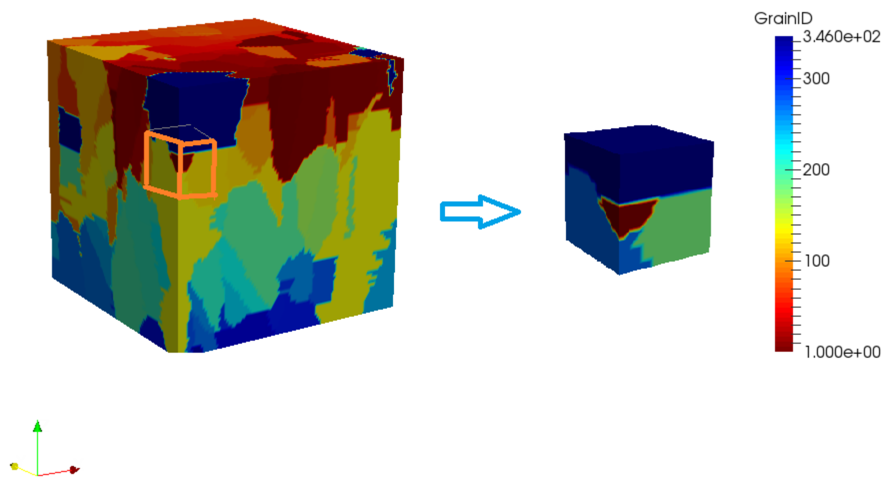

Figure 1: Input microstructure (3D Materials Atlas [2])

This is an illustrative example of a simple tension deformation problem. A real microstructure was tested with the material parameters of bcc β Ttitanium which were obtained from [1]

Input Parameters

```
/*FE parameters*/
#define feOrder 1 // Basis function interpolation order (1-linear)
#define quadOrder 2 // Quadrature point order n^3 (2->8 quadrature points)

/*Mesh parameters*/
//Set the length of the domain in all three dimensions
//Each axes spans from zero to the specified length
#define spanX 1.0
#define spanY 1.0
#define spanZ 1.0
// The number of elements in each direction is 2^(refineFactor) * subdivisions
// For optimal performance, use meshRefineFactor primarily to determine the
    element size
#define subdivisionsX 1
#define subdivisionsY 1
```

```
#define subdivisionsZ 1
#define meshRefineFactor 3 // 2^n*2^n*2^n elements(3->8*8*8 =512 elements)
#define writeMeshToEPS true //Only written for serial runs and if number of
    elements < 10000

/*Solution output parameters*/
#define writeOutput true // flag to write output vtu and pvtu files
#define outputDirectory "."
#define skipOutputSteps 0
#define output_Eqv_strain true
#define output_Eqv_stress true
#define output_Grain_ID true


/*Solver parameters*/
#define linearSolverType PETScWrappers::SolverCG // Type of linear solver
#define totalNumIncrements 100 // No. of increments
#define maxLinearSolverIterations 50000 // Maximum iterations for linear solver
#define relLinearSolverTolerance 1.0e-10 // Relative linear solver tolerance
#define maxNonLinearIterations 4 // Maximum no. of non-linear iterations
#define absNonLinearTolerance 1.0e-18 // Non-linear solver tolerance
#define relNonLinearTolerance 1.0e-3 // Relative non-linear solver tolerance
#define stopOnConvergenceFailure false // Flag to stop problem if convergence
    fails

/*Adaptive time-stepping parameters*/
#define enableAdaptiveTimeStepping false //Flag to enable adaptive time steps
#define adaptiveLoadStepFactor 0.5 // Load step factor
#define adaptiveLoadIncreaseFactor 1.25
#define succesiveIncForIncreasingTimeStep 10

//Elastic Parameters

double elasticStiffness[6][6]={{97.7e3, 82.7e3, 82.7e3, 0, 0, 0},
                               {82.7e3, 97.7e3, 82.7e3, 0, 0, 0},
                               {82.7e3, 82.7e3, 97.7e3, 0, 0, 0},
                               {0, 0, 0, 37.5e3, 0, 0},
                               {0, 0, 0, 0, 37.5e3, 0},
                               {0, 0, 0, 0, 0, 37.5e3}}; //     Elastic
                                   Stiffness Matrix -Voigt Notation (MPa)


//Crystal Plasticity parameters

#define numSlipSystems 12 //
#define latentHardeningRatio 1.4 //q1

double initialSlipResistance[numSlipSystems]= {200.0, 200.0, 200.0, 200.0, 200.0,
    200.0, 200.0, 200.0, 200.0, 200.0, 200.0, 200.0}; //CRSS of slip sytems
double initialHardeningModulus[numSlipSystems]= {1500.0, 1500.0, 1500.0, 1500.0,
    1500.0, 1500.0, 1500.0, 1500.0, 1500.0, 1500.0, 1500.0, 1500.0}; //Hardening
    moduli of slip systems
```

```
double powerLawExponent[numSlipSystems]= {1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
    1.0, 1.0, 1.0, 1.0}; // Power law coefficient
double saturationStress[numSlipSystems]= {500.0, 500.0, 500.0, 500.0, 500.0,
    500.0, 500.0, 500.0, 500.0, 500.0, 500.0, 500.0}; // Saturation stress


//Slip systems files
#define slipDirectionsFile "slipDirections.txt" // Slip Directions File
#define slipNormalsFile "slipNormals.txt" // Slip Normals File


// Crystal Plasticity Constitutive model parameters

#define modelStressTolerance 1.0e-6 // Stress tolerance for the yield surface
    (MPa)
#define modelMaxSlipSearchIterations 20 // Maximum no. of active slip search
    iterations
#define modelMaxSolverIterations 10 // Maximum no. of iterations to achieve
    non-linear convergence
#define modelMaxPlasticSlipL2Norm 0.8 // L2-Norm of plastic slip strain-used for
    load-step adaptivity
#define adaptiveLoadStepFactor 0.5 // Load step factor

//Read Input Microstructure
unsigned int numPts[3]={20, 20, 22}; // No. of voxels in x,y and z directions
#define grainIDFile "grainID.txt" // Grain ID File
#define headerLinesGrainIDFile 5 // No. of header Lines
#define grainOrientationsFile "orientations.txt" // Slip Normals File
```

References

[1] Lewis, Alexis C., Siddiq M. Qidwai, and Andrew B. Geltmacher. "Slip systems and initiation of plasticity in a body-centered-cubic titanium alloy." Metallurgical and Materials Transactions A 41.10 (2010): 2522-2531.

[2] 3D Materials Atlas AL6XN+Reconstruction

Table 1: BCC Titanium Slip Systems

System Number	Slip Direction	Slip Plane
1	[1 -1 1]	(0 1 1)
2	[1 1 -1]	(0 1 1)
3	[-1 1 1]	(1 0 1)
4	[1 1 -1]	(1 0 1)
5	[-1 1 1]	(1 1 0)
6	[1 -1 1]	(1 1 0)
7	[1 1 1]	(0 -1 1)
8	[-1 1 1]	(0 -1 1)
9	[1 1 1]	(1 0 -1)
10	[1 -1 1]	(1 0 -1)
11	[1 1 1]	(-1 1 0)
12	[1 1 -1]	(-1 1 0)
13	[1 1 -1]	(1 1 2)
14	[1 -1 1]	(-1 1 2)
15	[-1 1 1]	(1 -1 2)
16	[1 1 1]	(1 1 -2)
17	[1 -1 1]	(1 2 1)
18	[1 1 -1]	(-1 2 1)
19	[1 1 1]	(1 -2 1)
20	[-1 1 1]	(1 2 -1)
21	[-1 1 1]	(2 1 1)
22	[1 1 1]	(-2 1 1)
23	[1 1 -1]	(2 -1 1)
24	[1 -1 1]	(2 1 -1)
25	[1 1 -1]	(1 2 3)
26	[1 -1 1]	(-1 2 3)
27	[-1 1 1]	(1 -2 3)
28	[1 1 1]	(1 2 -3)
29	[-1 1 1]	(3 1 2)
30	[1 1 1]	(-3 1 2)
31	[1 1 -1]	(3 -1 2)
32	[1 -1 1]	(3 1 -2)
33	[1 -1 1]	(2 3 1)
34	[1 1 -1]	(-2 3 1)
35	[1 1 1]	(2 -3 1)
36	[-1 1 1]	(2 3 -1)
37	[1 -1 1]	(1 3 2)
38	[1 1 -1]	(-1 3 2)
39	[1 1 1]	(1 -3 2)
40	[-1 1 1]	(1 3 -2)
41	[1 1 -1]	(2 1 3)
42	[1 -1 1]	(-2 1 3)
43	[-1 1 1]	(2 -1 3)
44	[1 1 1]	(2 1 -3)
45	[-1 1 1]	(3 2 1)
46	[1 1 1]	(-3 2 1)
47	[1 1 -1]	(3 -2 1)
48	[1 -1 1]	(3 2 -1)