

PRISMS-Plasticity

Crystal Plasticity

Shear example -HCP AZ31 Mg alloy

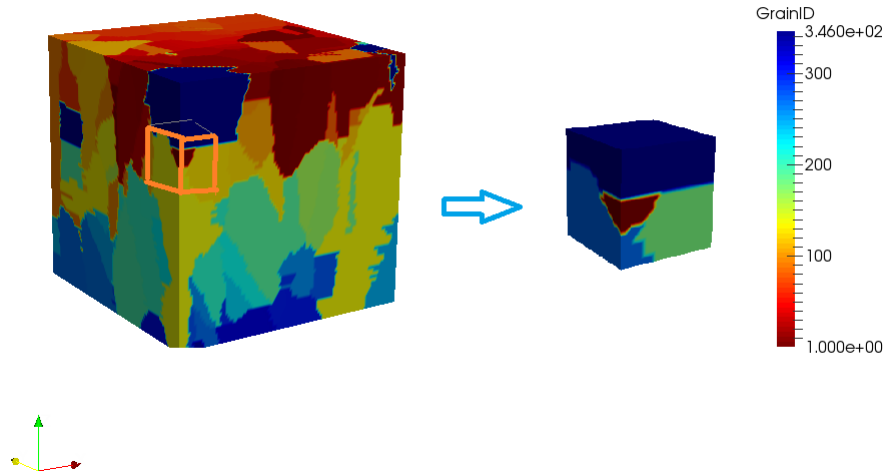


Figure 1: Input microstructure (3D Materials Atlas [2])

This is an illustrative example of a shear deformation problem. A virtual hcp microstructure was tested with the material parameters of AZ31 Mg alloy which were obtained from [1]

Input Crystal Parameters-parameters.h

```
//Elastic Parameters

#define c11 59.3e3 // C11 (MPa)
#define c12 25.7e3 // C12 (MPa)
#define c13 21.4e3 // C44 (MPa)
#define c33 61.5e3 // C33 (MPa)
#define c44 16.4e3 // C44 (MPa)

//Crystal Plasticity parameters

#define numSlipSystems 18 // No. of slip systems
#define numTwinSystems 6 // No. of twin systems
#define latentHardeningRatio 1.4 //q1
#define powerLawExponent1 1.1 //a_basal
#define powerLawExponent2 0.8 //a_prismatic
```

```

#define powerLawExponent3 0.8 //a_pyramidal<a>
#define powerLawExponent4 0.8 //a_pyramidal<c+a>
#define powerLawExponent5 1.1 //a_twin<c+a>
#define initialSlipResistance1 25.0 // CRSS s0_basal(MPa)
#define initialSlipResistance2 68.0 // CRSS s0_prismatic(MPa)
#define initialSlipResistance3 68.0 // CRSS s0_pyramidal<a>(MPa)
#define initialSlipResistance4 68.0 // CRSS s0_pyramidal<c+a>(MPa)
#define initialSlipResistance5 40.0 // CRSS s0_twin<c+a>(MPa)
#define saturationStress1 70.0 //s_s_basal(MPa)
#define saturationStress2 210.0 //s_s_prismatic(MPa)
#define saturationStress3 210.0 //s_s_pyramidal<a>(MPa)
#define saturationStress4 210.0 //s_s_pyramidal<c+a>(MPa)
#define saturationStress5 50.0 //s_s_twin<c+a>(MPa)
#define initialHardeningModulus1 100.0 //h0_basal(MPa)
#define initialHardeningModulus2 130.0 //h0_prismatic(MPa)
#define initialHardeningModulus3 130.0 //h0_pyramidal<a>(MPa)
#define initialHardeningModulus4 130.0 //h0_pyramidal<c+a>(MPa)
#define initialHardeningModulus5 50.0 //h0_twin<c+a>(MPa)

```

Input Geometry Parameters

```

// In main.cc crystalPlasticity<dim>::mesh()
double spanX=1.0; //Span along x-axis
double spanY=1.0; //Span along y-axis
double spanZ=1.0; //Span along z-axis

#define feOrder 1 // Basis function interpolation order (1-linear)
#define quadOrder 2 // Quadrature point order n^3 (2->8 quadrature
    points)
#define meshRefineFactor 3 // 2^n*2^n*2^n elements(3->8*8*8 =512
    elements)
#define totalNumIncrements 100 // No. of increments

//In main.cc class BCFunctor : public Function<dim>
values[0]=0.001; // displacement along X-Direction per increment

// Read Input Microstructure

unsigned int numPts[3]={20, 20, 22}; // No. of voxels in x,y and z
    directions

```

References

[1] Choi, S-H., et al. "Simulation of stress concentration in Mg alloys using the crystal plasticity finite element method." Acta Materialia 58.1 (2010): 320-329.

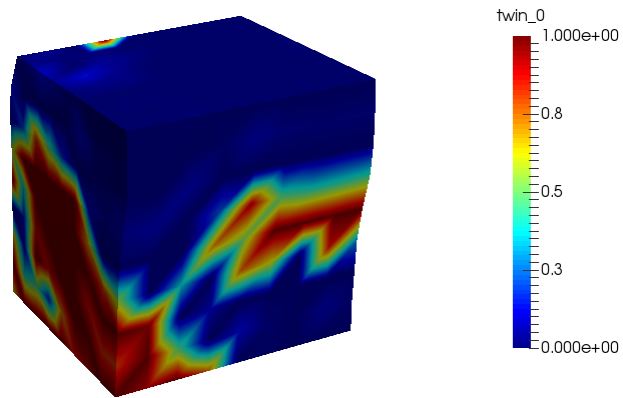


Figure 2: Twinned region(0-no twin, 1-twin) shown on a deformation field

[2] 3D Materials Atlas AL6XN+Reconstruction

Table 1: HCP Magnesium Slip Systems

System Number	Slip Direction	Slip Plane
1	$[1\ 1\ -2\ 0]$	$(0\ 0\ 0\ 1)$
2	$[-2\ 1\ 1\ 0]$	$(0\ 0\ 0\ 1)$
3	$[1\ -2\ 1\ 0]$	$(0\ 0\ 0\ 1)$
4	$[1\ -2\ 1\ 0]$	$(1\ 0\ -1\ 0)$
5	$[2\ -1\ -1\ 0]$	$(0\ 1\ -1\ 0)$
6	$[1\ 1\ -2\ 0]$	$(-1\ 1\ 0\ 0)$
7	$[1\ -2\ 1\ 0]$	$(1\ 0\ -1\ 1)$
8	$[-2\ 1\ 1\ 0]$	$(0\ 1\ -1\ 1)$
9	$[-1\ -1\ 2\ 0]$	$(-1\ 1\ 0\ 1)$
10	$[-1\ 2\ -1\ 0]$	$(-1\ 0\ 1\ 1)$
11	$[2\ -1\ -1\ 0]$	$(0\ -1\ 1\ 1)$
12	$[1\ 1\ -2\ 0]$	$(1\ -1\ 0\ 1)$
13	$[-1\ -1\ 2\ 3]$	$(1\ 1\ -2\ 2)$
14	$[1\ -2\ 1\ 3]$	$(-1\ 2\ -1\ 2)$
15	$[2\ -1\ -1\ 3]$	$(-2\ 1\ 1\ 2)$
16	$[1\ 1\ -2\ 3]$	$(-1\ -1\ 2\ 2)$
17	$[-1\ 2\ -1\ 3]$	$(1\ -2\ 1\ 2)$
18	$[-2\ 1\ 1\ 3]$	$(2\ -1\ -1\ 2)$
19	$[-1\ 0\ 1\ 1]$	$(1\ 0\ -1\ 2)$
20	$[1\ 0\ -1\ 1]$	$(-1\ 0\ 1\ 2)$
21	$[-1\ 1\ 0\ 1]$	$(1\ -1\ 0\ 2)$
22	$[1\ -1\ 0\ 1]$	$(-1\ 1\ 0\ 2)$
23	$[0\ -1\ 1\ 1\ 1]$	$(0\ 1\ -1\ 2)$
24	$[0\ 1\ -1\ 1]$	$(0\ -1\ 1\ 2)$