**GB Generation Variables**

|  |  |
| --- | --- |
| Lattice | GB\_Grain\_Rot.m GB\_SymOp.m |
| Basis | GB\_Grain\_Rot.m GB\_SymOp.m |
| Species | GB\_Grain\_Rot.m GB\_WriteFiles.m |
| Masses | GB\_Grain\_Rot.m GB\_WriteFiles.m |
| Axis | GB\_Grain\_Rot.m |
| Direction | GB\_Grain\_Rot.m |
| MaxMiller | GB\_Grain\_Rot.m |
| Verbose | GB\_Grain\_Rot.m GB\_Orientations.m GB\_Construct.m |
| Dis\_Tol | GB\_Grain\_Rot.m |
| Deg\_Tol | GB\_Grain\_Rot.m |
| Symmetry | GB\_Grain\_Rot.m GB\_SymOp.m |
| Sym\_Tol | GB\_Grain\_Rot.m GB\_SymOp.m |
| GrainRot(1/2) | GB\_Orientations.m |
| Strain\_Tol | GB\_Orientations.m |
| MaxArea | GB\_Orientations.m |
| nGBs | GB\_Construct.m |
| GBSort | GB\_Construct.m |
| WriteStyle | GB\_Construct.m |
| Overlap\_Tol | GB\_Construct.m |
| NormSlabDim | GB\_Construct.m |
| Vacuum | GB\_Construct.m |
| GBregion | GB\_Construct.m |
| FullyPeriodic | GB\_Construct.m |
| Suffix | GB\_Construct.m |
| Orientation | GB\_SymOp.m |
| GBorientations | GB\_Construct.m GB\_Bulk.m |
| File\_Base\_id | GB\_WriteFiles.m |
| Write\_Style | GB\_WriteFiles.m |
| AtomData | GB\_WriteFiles.m GB\_WrapPBC.m |
| Header | GB\_WriteFiles.m |
| Archive | GB\_WriteFiles.m GB\_Bulk.m |
| Dir\_Base | GB\_WriteFiles.m GB\_Bulk.m |
| MaxEdge | GB\_WrapPBC.m |
| PBC\_Overlap\_Tol | GB\_WrapPBC.m |
| vars | GB\_Vars.m |
| Fun | GB\_Vars.m |
| Write\_Style | GB\_Bulk.m |

**GB Generation Codes**

**Active**

***GB\_Grain\_Rot.m***

This scipt deterimines all possible grain rotations along a specified Axis for a givin Lattice. The script insures that all rotations are mapped onto an orthogonal set of vectors as it searches across hkl values of +/- MaxMiller. The specified Axis is alligned along the Direction of choice (in the simulation reference frame). Each grain rotation is compared to identical grain rotations as related by the computed symmetry for the Lattice and Basis.

GrainRot=GB\_GrainRot(Lattice,Basis,Species,Masses,Axis,Direction,MaxMiller,Dis\_Tol,Deg\_Tol,Symmetry,Sym\_Tol,Verbose)

***GB\_Orientations.m***

[GBorientations,id\_Area,id\_Angle]=GB\_Orientations(GrainRot1,GrainRot2,Strain\_Tol,MaxArea,Verbose)

***GB\_Construct.m***

GB\_Construct(GBorientations,nGBs,GBSort,WriteStyle,Overlap\_Tol,NormSlabDim,Vacuum,GBregion,FullyPeriodic,Suffix,Verbose)

**Supportive**

***GB\_SymOp.m***

[ActiveSymmetry,NSymmetry] = GB\_SymOp(Lattice,Basis,Symmetry,Orientation,Sym\_Tol)

***GB\_WriteFiles.m***

GB\_WriteFiles(File\_Base\_id,Write\_Style,AtomData,Species,Masses,Corners,Header,Archive,Dir\_Base,Verbose)

***GB\_WrapPBC.m***

[AtomData,nPBC\_overlap]=GB\_WrapPBC(AtomData,MaxEdge,PBC\_Overlap\_Tol)

***GB\_Bulk.m***

GB\_Bulk(GBorientations,Write\_Style,Archive,Dir\_Base,Verbose)

***GB\_Vars.m***

vars\_pass = GB\_Vars(vars,fun)

GB\_FillRegion.m

AtomData=GB\_FillRegion(Lattice,Basis,Orientation,Lx,Ly,Lz,TypeOffset)