MedeA Microstructure Builder

Build Complex Grain Structures

At-a-Glance

The *MedeA* ®[1] *Microstructure Builder* creates realistic polycrystalline grain structures, arbitrary interfaces and nanocrystals.

Key Benefits

- *Automatic building of simple or complex grain structures*
- *Straightforward interactive model construction*

Creating realistic microstructure models is a prerequisite to understanding materials' behavior, predicting materials' properties, and optimizing materials' performance. Properties such as strength, ductility, conductivity, and reactivity of realistic materials are directly influenced by a materials' microstructure. By manipulating the microstructure, material performance can be optimized, e.g., the grain size in a polycrystalline material can be tailored to improve its mechanical properties. The *MedeA Microstructure Builder* can create atomic structures for metals, semiconductors, or ceramics, whereas organic systems are better handled by the *MedeA Amorphous Builder* module.

The *Microstructure Builder* generates atomistic grain structures composed of user-specified phases using a *Seed & Growth* algorithm developed at Materials Design. In this algorithm, seed points are either placed randomly or at user-specified coordinates in the supercell. Each seed point is then used as an origin to grow a grain by placing atoms from that seed point outwards until the grain boundary is reached. The beginning user only needs to specify the components and number of grains per component, where a component is any periodic unit cell. An example is shown in the top panel of the figure below for a Cu-Ag grain structure. The building of the microstructure is carried out interactively, with the resulting structure appearing in the graphical interface when the built is complete.

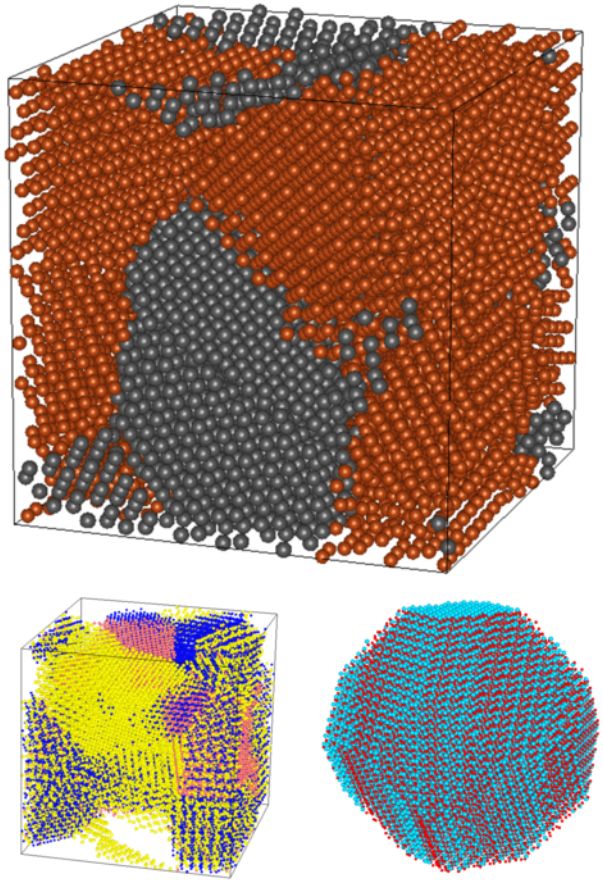

Fig. 1: Examples of atomistic models built with the Microstructure Builder. *From top to bottom and left to right: A Cu-Ag multicrystalline grain structure, polycrystalline $Li_{10}GeP_2S_{12}$, Li, Ge, and P multi-phase grain structure with voids ready to be sintered, and a ZrO_2 nanocrystal.*

Several growth parameters can be adjusted by an intermediate user. First, the user can enable and change the default thresholds on interatomic distances. Without such a threshold, atoms from different grains might be placed arbitrarily close to each other at the grain boundary in the *Seed & Growth* algorithm. Second, the user can specify whether the grains should grow stoichiometrically. In that case, the number of atoms of each species in the grain is proportional to the number of atoms of that species in the unit cell. Third, slab structures can be easily generated by switching to the

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slab-growth mode, with full control over slab thickness and composition.

Advanced usage allows for the creation of porous microstructures, as seen in the bottom left panel of the figure. The *Microstructure Builder* can also be used for the generation of interfaces with complex and irregular shapes or nanocrystals of complex shapes, as shown in the bottom right panel of the figure. In addition, interstitial atoms can be inserted at the grain boundaries. An optional analysis feature is available to calculate the grain sizes, centroid distances or misorientation angles in the resulting microstructure.

The resulting models are fully periodic and can be used directly with the *MedeA LAMMPS* module. Additionally, the user can further edit the structures in their *MedeA* client to introduce impurities, vacancies, and interstitial atoms as needed. Voids can be populated in a subsequent step with the *MedeA Docking* module. We also recommend the *MedeA Interface Builder* which offers more control over the interface in simpler slab geometries.

Key Features

- Choose any periodic unit cell as a component
- Use any number of components and grains
- Control interatomic distances at grain boundaries
- Grow grains preserving the component's stoichiometry
- Change interatomic-distances thresholds, seed point coordinates, and grain rotations

Required Modules

- *MedeA Environment*

Recommended Modules

- *MedeA LAMMPS*
- *MedeA Docking*
- *MedeA Interface Builder*

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