BIOVIA MATERIALS STUDIO AMORPHOUS CELL

DATASHEET

What Does BIOVIA Materials Studio Amorphous Cell Do? BIOVIA Materials Studio Amorphous Cell is a comprehensive model building tool for creating a wide range of amorphous materials. Its flexible[1] approach to forcefield choice, combined with several different construction techniques, enables the building of a bulk structures of a wide range of systems including polymers and glasses, as well as nanostructures. BIOVIA Materials Studio Amorphous Cell can also be used to generate layered structures to enable calculations on interfaces.

KEY USES OF BIOVIA MATERIALS STUDIO AMORPHOUS CELL

The behavior of amorphous materials is critical to products such as plastics, glasses, foods, and chemicals. Researchers studying amorphous polymers, for example, seek to optimize their mechanical behavior, the transport of molecules through the system, and their surface and interface interactions. These properties impact the polymer's performance in applications such as separation processes, packaging, and drug delivery.

Polymers

Building accurate models of polymers is key to predicting the properties of these materials. BIOVIA Materials Studio Amorphous Cell has been designed to build realistic models of chain molecules enabling fast prediction of properties such as density, mechanical properties, and diffusivity. Combine models of small molecules such as drugs, with the polymer models to predict compatibility.
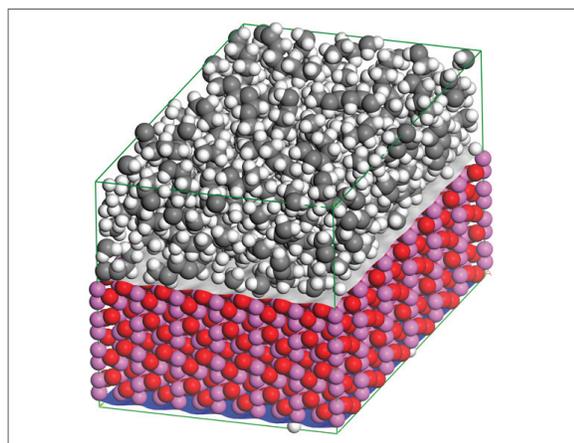

Figure 1: BIOVIA Materials Studio Amorphous Cell allows packing of molecules into nonorthogonal cells, enabling simulations of solvents on cleaved surfaces.

Inorganic glasses

Use specialised forcefields to construct initial starting structures for inorganic glassy materials. These can be further used with other classical simulations modules such as BIOVIA Materials Studio Forcite Plus and BIOVIA Materials Studio GULP to predict key properties.

Solvation of systems

Use the "Packing" task to soak molecules or surfaces with a solvent. Use the classical simulations modules to predict interaction energies between surfaces and solvents.

HOW DOES BIOVIA MATERIALS STUDIO AMORPHOUS CELL WORK?

In BIOVIA Materials Studio Amorphous Cell, molecules are added into a three-dimensional box by growing the candidate molecules inside the box segment by segment, taking into account interaction with all atoms already positioned, whilst continuously monitoring the single chain conformations. After each head segment is placed, the chain molecules are grown by selecting the next segment from a number of candidate structures. Each of the candidate structures is subjected to a number of checks such as ring spearing and close contacts. For the candidates that pass the initial tests, a probability, based on the energy of adding the segement, is calculated. These are compared to a random number and the next candidate is chosen.

The result of this sampling method is that low energy sites are preferred over high energy sites. Using this method, BIOVIA Materials Studio Amorphous Cell generates bulk disordered systems containing chains molecules in realistic equilibrium conformations[1].
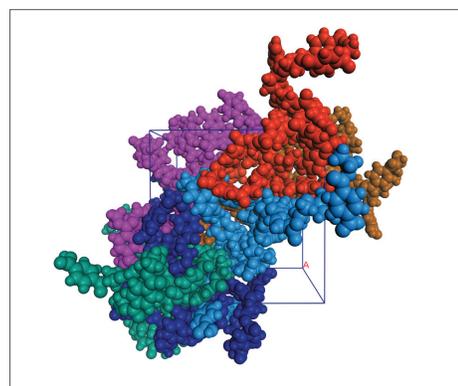

Figure 2: Polymers with rigid backbones such as polyethylene terepthalate can be packed into cells at experimental densities.

BIOVIA MATERIALS STUDIO INTEGRATION

BIOVIA Materials Studio Amorphous Cell is operated from within the BIOVIA Materials Studio environment. A flexible client-server architecture means that BIOVIA Materials Studio Amorphous Cell calculations can be run on servers located elsewhere on your network.
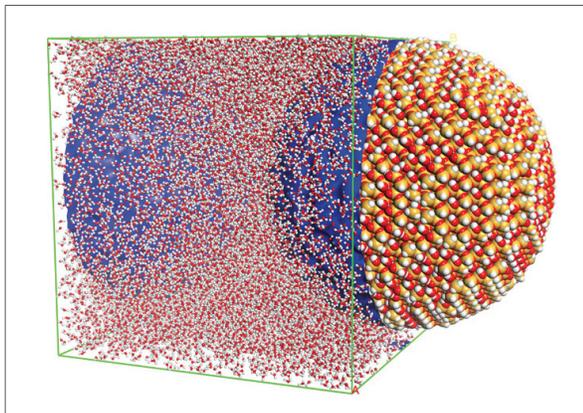

Figure 3: The packing task enables fast solvation of existing structures such as this nanoparticle of silica.

To use the program, you begin with the molecular structure of the polymer or material you wish to study, which can be constructed using BIOVIA Materials Studio Visualizer's polymer building and sketching tools or loaded from a database. You then set simulation parameters, including system composition and density, and BIOVIA Materials Studio Amorphous Cell constructs a periodic model of the system for you.

The resulting amorphous cell can be used with classical and quantum simulations for property prediction. You can also use the coarse-graining tools to generate bead representations of the amorphous materials for use in mesoscale modeling.

FEATURES AND CAPABILITIES

General Model Building

- Flexible building algorithm
  - Model building using a modified Markov process[2] with bond conformational probabilities chosen to account for both intramolecular and intermolecular non-bonded interactions
  - Fast model building using a geometrical close contact check
  - Combined build with both energy and close contact check

- Flexible torsion definition:
  - Backbone atoms in polymer chains
  - All flexible torsions
  - Torsions defined on the model
- Ring spearing and catenation checks.
- Set temperature to control ability to build higher energy conformations.
- Modify number of bonds that are used to generate candidate
- structures.
- Control the number of attempts to add molecules into the cell.
- Optimization of the new amorphous cell after construction.

Energy options

- Support for Universal, BIOVIA Materials Studio Compass, Dreiding, PCFF, CVFF or customized forcefields.
- Charging using forcefield defined charges, Qeq or Gasteiger methodologies.

Construction task

- Construct an amorphous cell at a set density using one or more input molecules.
- Specify loading as number of molecules.
- Build at a specific density or ramp to a target density.
- Build cubic, tetragonal or orthorhombic cells.

Packing task

- Pack one or more molecules into a volume at a specified density.
- Specify loading by the molar ratio of the molecules.
- Pack into:
  - non-orthogonal cells
  - cells already containing atoms
  - isosurfaces

Confined layer task

- Construct an amorphous cell at a set density with the molecules confined to a layer.
- Specify loading as number of one or more molecules.
- Build cubic, tetragonal, or orthorhombic cells.
- Choose to confine along A, B or C lattice vectors.

To learn more about BIOVIA Materials Studio, go to **accelrys.com/materials-studio**

REFERENCES:

1. Theodorou, D.N. and Suter, U.W., Macromolecules, 1985, 18, 1485; 1986, 19, 139.

2. Allen, M.P. and Tildesley, D.J., Computer Simulation of Liquids, Oxford University Press, 1987.

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