

Sophisticated construction, simulation, and analysis of amorphous systems

Flexible protocols for applying complex simulation strategies

Powerful analysis tools to examine many properties of resulting structures

Amorphous Cell

Amorphous Cell is a comprehensive set of model construction, simulation, and analysis tools for predicting properties of amorphous systems. 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.

What Does Amorphous Cell Do?

Amorphous Cell is a suite of computational tools that allow you to construct representative models of complex amorphous systems and predict key properties. By observing the relation between system structure and properties, you can obtain a more thorough understanding of the important molecular features, allowing for a better design of new compounds or new formulations. Among the properties that you can predict and investigate are cohesive energy density, equation-of-state behavior, chain packing, and localized chain motions.

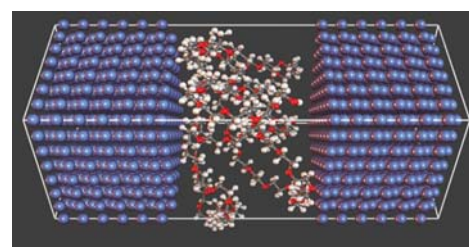
The methodology of Amorphous Cell construction is based on an extension of well-established methods for generating bulk disordered systems containing chain molecules in realistic equilibrium conformations¹. Other features include provision for construction of arbitrary mixture systems containing any combination of small molecules and polymers, in addition to special capabilities for producing ordered nematic mesophases and slabs of amorphous material suitable for use in creating models of interphases and confined fluids, as would be required to study adhesion, lubrication, and shear viscosity.

The Materials Studio Advantage

Amorphous Cell is operated from within Materials Studio's MS Modeling environment. Materials Studio provides a user interface that is easy-to-use and quick to learn, complying with Windows® standards. Materials Visualizer, the core Materials Studio product, offers a wide range of model

building and visualization tools. A flexible client-server architecture means that Amorphous Cell calculations can be run on servers located elsewhere on your network.

To use the program, you begin with the molecular structure of the polymer or material you wish to study, which can be constructed using Materials Visualizer's polymer building and sketching tools or loaded from a database. You then set simulation parameters, including system composition and density, and Amorphous Cell constructs a periodic model of the system for you. The program interfaces with the Discover® simulation product to perform structure minimization and further extend the range of available simulation and analysis options.



A polyoxyethylene oligomer confined between two iron surfaces. Such a scenario can be used to study the effect of shear on the polymer structure and properties.

Features

- Model construction using a modified Markov process² with bond conformational probabilities chosen to account for both intramolecular and intermolecular non-bonded interactions
- Optional energy minimization of the bulk model
- Molecular dynamics simulations at constant temperature and density, or under other commonly encountered conditions such as constant temperature and pressure, to yield predictions of PVT relations
- Full support for the state-of-the-art COMPASS force field
- Flexible protocols for applying complex simulation strategies, including:
 - Confined shear simulation for study of lubrication and viscosity³
 - Poling to study electric polarization and dielectric behavior
 - Temperature cycling protocol for studying response to heating and cooling cycles
 - Hybrid Monte Carlo alternative to traditional molecular dynamics simulation⁴
- Powerful analysis tools to examine many properties of the resulting structures, including:
 - Cohesive energy density/solubility parameter⁵
 - All aspects of molecular/chain geometry (either global, or localized within specified chemical groupings) over a dynamics trajectory chain
 - Configurational statistics for properties such as end-to-end distances and radii of gyration
 - Atom-atom pair correlation functions⁶
 - X-ray or neutron scattering curves
 - Gas/small molecule diffusivities (via mean-square atom displacements or velocity autocorrelation functions)
 - Infrared spectra and dipole correlation functions
 - Elastic stiffness coefficients⁷
 - Surface properties.

System Requirements:

For Materials Studio system requirements see www.accelrys.com/products/mstudio/sysreqs.html

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**.
3. Khare, R., de Pablo, J., and Yethiraj, A., *J. Chem. Phys.*, **2001**, *114*(17), 7593-7601.
4. Mehlig, B., Heerman, D.W., and Forrest, B. M., *Phys. Rev.*, **1992**, *B45*, 679.
5. Hildebrand, J.H. and Wood, S.E., *J. Chem. Phys.*, **1933**, *1*, 817.
6. Rigby, D. and Roe, R.J., *J. Chem. Phys.*, **1988**, *89*, 5280.
7. Brown, D. and Clarke, J.H.R., *Macromolecules*, **1991**, *24*, 2075; Parrinello, M. and Rahman, A., *J. Chem. Phys.*, **1982**, *76*, 2662; Theodorou, D. N. and Suter, U.W., *Macromolecules*, **1986**, *19*, 139.