BIOVIA MATERIALS STUDIO MESOPROP

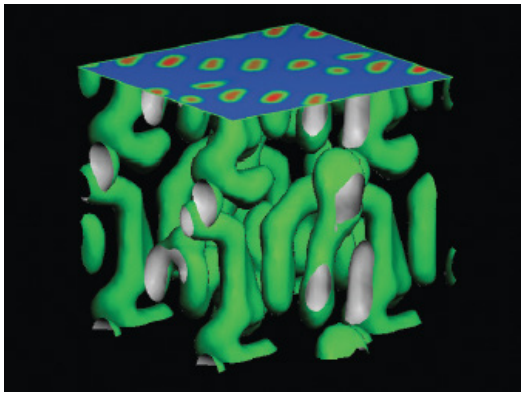
DATASHEET

BIOVIA Materials Studio MesoPROP is a new research tool which is used to predict the bulk properties of multicomponent nanostructured materials systems. The research applications for BIOVIA Materials Studio MesoPROP include studies of polymers, surfactants and continuous phases which are fundamental to the development of surface coatings, adhesives, sealants, elastomers, cements, composite materials, gels, and laminates.

BIOVIA Materials Studio MesoPROP is a fully integrated research tool which links the properties of pure components to complex blends. Applications include formulation and simulation studies of block copolymers, polymer surfactants, nanostructured polymer blends, and physical effects at interfaces such as membranes.

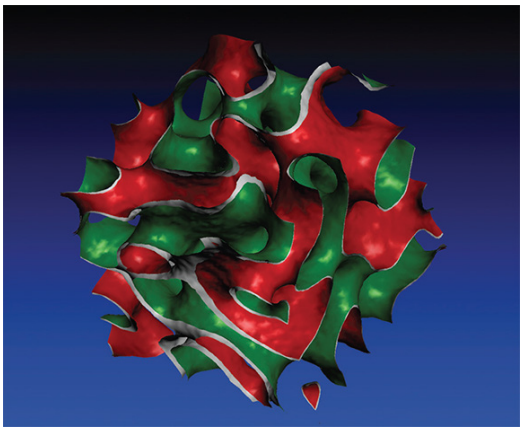
BIOVIA Materials Studio MesoPROP offers:

- Predictive studies to streamline research projects and save costs
- Faster product development and shorter time to market
- A business tool for cost engineering: optimizing raw materials usage and reducing formulation costs
- A systematic approach to process and product development, a wide range of input and output information can be captured and held for future use or later inspection.



HOW DOES BIOVIA MATERIALS STUDIO MESOPROP WORK?

BIOVIA Materials Studio MesoPROP uses the complex phase morphologies from the MS Modeling MesoDyn and DPD codes to give a dynamic simulation of complex fluid systems at the mesoscale level. The researcher then selects input data of pure components from the BIOVIA Materials Studio MesoPROP database. BIOVIA Materials Studio MesoPROP then introduces property calculations using Finite Element Analysis algorithms to produce visual models and output data.

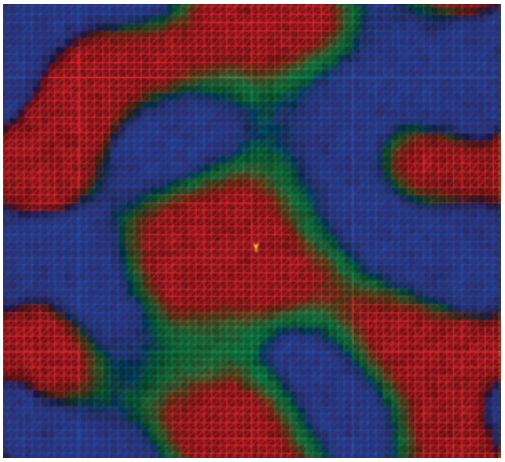


The core algorithms and input databases include:

- Elastic constants (stiffness and compliance)
- Thermal expansion coefficients
- Thermal conductivity
- Electrical conductivity
- Dielectric constants
- Gas diffusion constants.

If the physical property is not covered in the BIOVIA Materials Studio MesoPROP database, then MS Modeling polymer property predictor Synthia can be used to to calculate:

- Refractive index
- Magnetic moments
- Swelling in solvents
- Liquid diffusion
- Liquid permeability.



FEATURES AND CAPABILITIES

- A practitioners tool for technicians, engineers, and formulation chemists
- Provides cost saving solutions for new product and process development
- Uses desktop IT equipment in an office environment, reduces the need for 'live' experiments in wet labs and clean rooms
- Versatile software package, applicable to up to 10 separate chemical components
- Fast turnaround, several projects can be processed simultaneously. Results displayed for presentations and transferred electronically
- Developed for demanding and highly regulated process industries
- Potential to link BIOVIA Materials Studio MesoPROP to production and process engineering software.

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

REFERENCES:

The following list of scientific papers relate to the methods used in BIOVIA Materials Studio MesoPROP and some practical applications:

1. A. A.Gusev, "Representative Volume Element Size for Elastic Composites:A Numerical Study," J. Mech. Phys. Solids 45(9), 1449-1459 (1997).
2. O. A. Goussev, P. Richner, M. G. Rozman,A.A. Gusev, "Void-containing materials with tailored Poisson's ratio," J. Appl. Phys. 88(7), 4013-4016 (2000).
3. A.Gusev, P. J.Hine, I.M.Ward, "Fiber packing and elastic properties of a transversely random unidirec tional glass/epoxy composite," Comp. Sci. Techn. 60, 535-541 (2000).
4. A. A.Gusev, J. J. M. Slot, "Non-Additive Morphology Effects in Thermal Expansion of Three-Phase Materials," Adv. Eng. Mater. 3(6), 427-427 (2001).
5. A. A.Gusev, H. R. Lusti, "Rational Design of Nanocomposites for Barrier Applications," Adv. Mater. 13(21), 1641-1643 (2001).
6. M.Wissler, H. R. Lusti, C. Oberson, A. H.Widmann- Schupak, G. Zappini, A. A.Gusev, "Non-additive effects in the elastic behavior of dental composites," Adv. Eng. Mater. 5(3), 113-116 (2002).
7. A. A.Gusev, "Finite Element Mapping for Spring Network Representations of the Mechanics of Solids," Phys. Rev. Lett. 93(3), 034302-1-4 (2004). 8.O.Guseva, H. R. Lusti, A. A.Gusev, "Matching thermal expansion of mica-polymer nanocomposites and metals," Modelling Simul. Mater. Sci. Eng 12, 101-105 (2004).

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