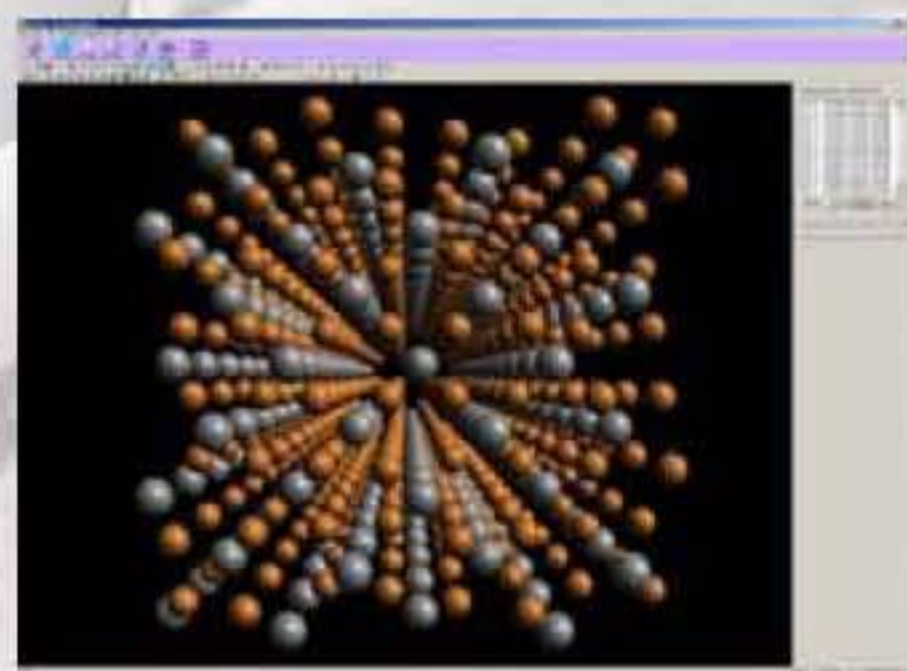


Materials Explorer[®]

Materials Explorer is a multi-purpose molecular dynamics (MD) software package for Windows-based computers. Intuitive graphical interface and sets of wizards make it simple to build assemblies of molecules in a cell, to set up calculations, and to interpret results. Materials Explorer can be applied to systems including metals and inorganics, such as ceramics and semi-conductors. It is also well suited for organics and biomolecules. Materials Explorer has a Potential Library that includes potential functions and parameters for a wide range of atom-atom interactions.

Handles most materials

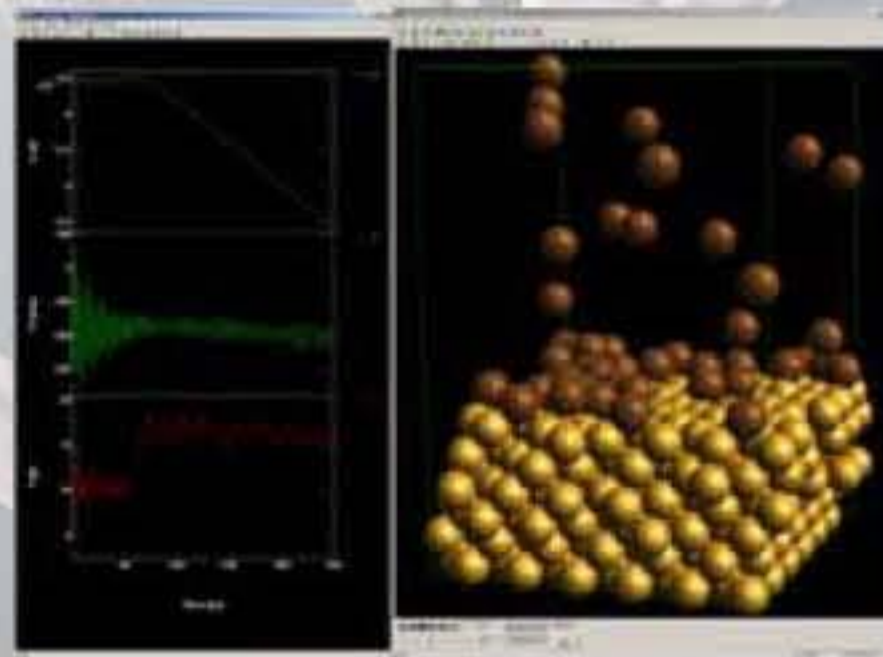
- Potential Force Field for Atom-to-Atom Interactions.
- Potential Library includes force fields (including 2Body, 3Body and EAM potentials) covering crystals, metals, ceramics, semi-conductors, solutions, liquids, gases, organic systems, polymers and biomolecules.
- Potential Editor manages the entry of and access to potential forms and parameters in the Potential Library.



Powerful Molecular Dynamics Engine

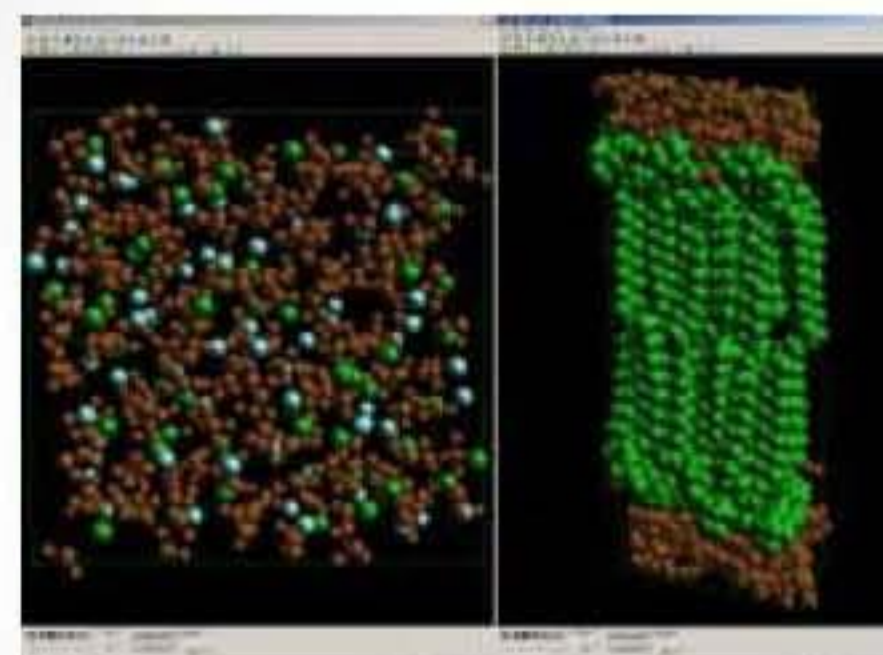
- Ensembles: NEV, NTV, NPH and NTP.
- The time evolution of the equations of motion is determined by Gear or Hernandez methods.
- Temperature and pressure - controlled MD simulations through employment of Parrinello-Rahman and Nose methods.

- SHAKE algorithm for stretch-bond constraint.
- Rigid-body treatment for small molecules.
- Periodic boundary conditions available.
- Initial relaxation - prevents explosion in liquid/amorphous simulation.
- External fields: electrostatic, magnetic, gravitational, containing sphere and elastic energy correction.
- Charges Definition Tool - determines the atomic charges of the molecule.



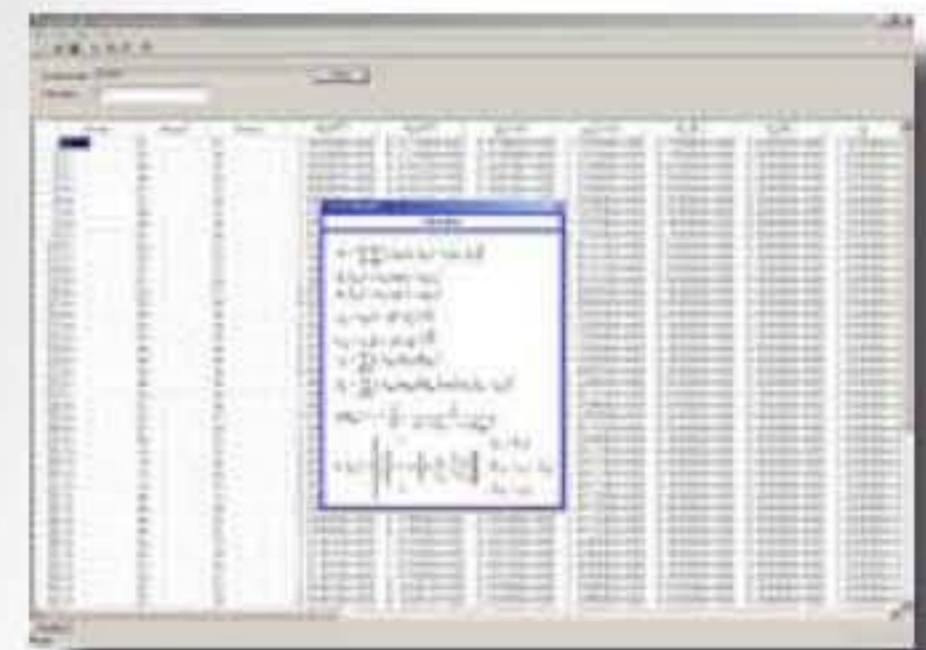
Analysis Modules

- Monitoring Module shows 2D graphs of temperature, pressure, internal energy, kinetic and potential energies, thermal conductivity and other thermodynamic properties.
- 3D Atomic Configuration Module displays the snapshot, trajectory, and animation of collective atomic configurations.
- MSD Module calculates the mean square displacement (MSD) from the output data. It also displays a 2D graph of the MSD, and the self-diffusion coefficient of each molecule.
- PCF Module calculates the pair correlation function, radial distribution function, and



running integration number, and displays the corresponding 2D graphs.

- Interference Function Module calculates X-ray and neutron diffraction based on the pair correlation function.
- Voronoi Module calculates the number of Voronoi polyhedra and the number of faces (polygons) of Voronoi polyhedra.
- Internal Coordinate Module calculates the bond lengths, bond angles, dihedral angles, or out-of-plane angles of the specified molecule type and displays the distribution in a histogram.
- Velocity Auto-Correlation Function & Spectrum Module calculates auto-correlation function and the spectrum based on Wiener-Khintchin's theorem.
- Modulus of Elasticity Module calculates modulus of elasticity from the fluctuation formula.



Hardware and software requirements

- Suggested hardware configuration: Intel Pentium 4 2.0 GHz or higher, 512 MB RAM or more, 500 MB HDD space or more.
- Operating Systems: Windows 98/ME/2000/XP.
- Materials Explorer computes engines are available on Linux machines (serial and parallel).