Molecular dynamics simulations of materials

What is MD?

Molecular dynamics involves the numerical solution of the classical equations of motion (F=ma) for every single atom in material. The result is a very detailed description of the temporal evolution of the material: we obtain the position, velocity and force of every atom as a function of time. The total force acting on an atom comes from its interaction with other atoms and external fields and an accurate model to describe atomic interactions is critical in any MD simulation. If you are interested in MD read on; you will find more information, additional resources, simulation codes, and online tool that enables running live MD simulations using simply your web-browser.

Advantages

As compared with other materials simulation techniques, MD exhibits several advantages: The only inputs to the simulation are the interatomic potential used to compute forces on atoms and the initial configuration; all other properties and processes are derived. For example, you cannot dial-in the melting temperature, or the character of the slip planes that will be activated during deformation, how a dislocation might look, nucleate or move, or how phonons interact with each other or with other defects. Consequently, phenomena like size effects in the thermal or mechanical response of materials are naturally captured by MD making a power technique in nanoscience and nanotechnology.

Approximations

MD is not without approximations and it is important to understand them in order to design meaningful simulations and correctly interpret their results. There are two key approximations:

1. Atomic interactions are now known exactly, and an accurate model to describe them is critical in MD simulations of realistic materials. Atomic forces can be obtained from *ab initio* electronic structure calculations (such as density functional theory); these methods provide accurate results (not exact) but are computationally intensive. Most MD simulation use of interatomic potentials (or force fields) that describe atomic interactions in terms of functions parameterized to describe specific materials using experimental or *ab initio* data. These potentials are less accurate and less transferable than *ab initio* calculations but are computationally less intensive enabling large-scale simulations (up to billions of atoms in current petaFLOP supercomputers).
2. Being based on classical mechanics, MD does not capture quantum effects on ionic dynamics. These effects originate when atomic vibrations around a minimum lead confinement of position and velocity that violates Heisenberg's uncertainty principle are important when simulations are performed at temperatures below or near the Debye temperature of the material.

Learn more about MD at nanoHUB.org

- *An Introduction to Molecular Dynamics.* A lecture series by Alejandro Strachan. Video, voiced-over presentations and notes: http://nanohub.org/resources/5838
- *Overview of Computational Nanoscience: a UC Berkeley Course.* By Jeffrey C Grossman, Elif Ertekin. Class notes in pdf format: https://nanohub.org/resources/3944
- *Short Course on Molecular Dynamics Simulation.* By Ashlie Martini. Class notes in pdf format: https://nanohub.org/resources/7570

Online MD simulations at nanoHUB.org

The **nanoMATERIALS simulation tool** https://nanohub.org/resources/matsimtk enables running live MD simulations in nanoHUB.org. A simple-to-use graphical interface allows users to set up the initial structure, simulation conditions (e.g. thermodynamic ensemble, temperature, strain rate), and output options; advanced options enable users to compute thermal conductivity using non-equilibrium simulations.

Learn more about the **nanoMATERIALS simulation tool** and run simulations via the following tutorials:

- *Running MD on the nanoHUB: The nano-MATERIALS Simulation Toolkit.* http://nanohub.org/resources/5843
- *Materials strength: does size matter? nanoMATERIALS simulation toolkit tutorial.* https://nanohub.org/resources/2322

MD in research and education

- *First Principles-based Atomistic and Mesoscale Modeling of Materials.* https://nanohub.org/resources/434
- *Learning Module: Atomic picture of plastic deformation in metals.* Teach and learn about the atomic level mechanisms that govern plastic deformation is metals: https://nanohub.org/topics/LearningModulePlasticityMD

Other resources

Some of my favorite books and publications on MD

- Allen, M. P. and D. J. Tildesley. 1989. *Computer Simulation of Liquids*. Oxford (UK): Oxford University Press.
- Frenkel, Daan and Berend Smit. 2002. *Understanding Molecular Simulation: From Algorithms to Applications*. 2nd ed. San Diego: Academic Press..

Downloadable, free of charge, MD codes

- LAMMPS, the Large-scale Atomic/Molecular Massively Parallel Simulator from Sandia National Labs, is available at: http://lammps.sandia.gov/ .
- NAMD, from the University of Illinois at Urbana Champain, available at:

http://www.ks.uiuc.edu/Research/namd/

- GROMACS, GROningen MAchine for Chemical Simulations, is available at: http://www.gromacs.org/

Related codes and resources

- VMD, molecular visualization, http://www.ks.uiuc.edu/Research/vmd/