SAND2016-10721PE

*Exceptional service in the national interest*

Sandia National Laboratories

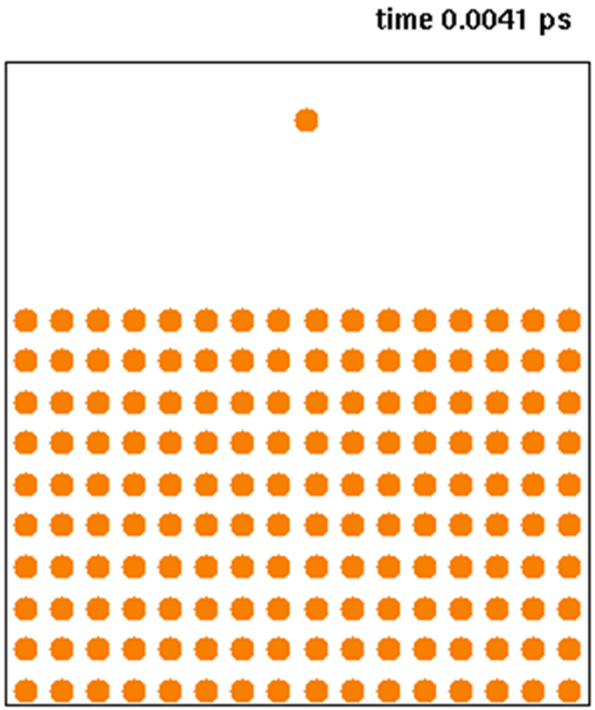
# Effects of Single Ion Strikes into Si on the 3D Reciprocal Space

Manuel Franco, Remi Dingreville, Khalid Hattar, Wei Ji

U.S. DEPARTMENT OF ENERGY

National Nuclear Security Administration

Sandia National Laboratories is a multi-mission laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND NO. 2011-XXXXP




Example of a molecular dynamics simulation in a simple system: deposition of one copper (Cu) atom on a Cu Miller index (001) surface. Each circle illustrates the position of one atom. The atomic interactions used in current simulations are more complex than those of 2-dimensional hard spheres. [1]

[1] Molecular Dynamics Wikipedia Gif Image

- What is MD for and why is it done?
  - Basic principles begin with classical MD
    - Approximate interatomic behavior and know beforehand the energy potentials
      - Based off of empirical data or independent structure calculation
    - Systems under investigation are limited in complexity
      - Though in comparison to other methods are quick and easy
  - Most often used in biochemistry/physics and materials science
  - Not Monte Carlo, MD is deterministic

Marx, Dominik; Hutter, Jurg; Ab Initio molecular dynamics: Theory and Implementation
Ootani, Y; An Introduction to Ab Initio Molecular Dynamics Simulations
Kuhne, Thomas; Ab-Initio Molecular Dynamics

- Ab-initio MD, what is it and how does it work
  - Means from the beginning
  - Refinement of MD meant to allow for more degrees of freedom
    - Quantum chemistry
    - Means more complicated systems can be solved
  - Subcategories exist here that vary in computational intensity
    - Ehrenfest
    - Car-Parrinello
    - Born-Oppenheimer
  - Most successful version is considered to be Density Functional Theory

[1]Marx, Dominik; Hutter, Jurg; Ab Initio molecular dynamics: Theory and Implementation
[2] Ootani, Y; An Introduction to Ab Initio Molecular Dynamics Simulations
[3] Kuhne, Thomas; Ab-Initio Molecular Dynamics

Sandia National Laboratories

## Classical MD

- Deterministic
- Relatively easy computationally

## Ab-Initio MD

- Introduces more freedom
- Involves much more computational resources

# Acknowledgements

This research was partially funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering. Sandia National Laboratories is a multi-program laboratory operated by the Sandia Corporation, a wholly owned subsidiary of Lockheed Martin company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.