

## Term project

**Objective:** To get experience in designing and performing computer simulations.

### **Parts of the project:**

- Design (or adapt an idea from literature) a simulation that is of scientific or computational interest to you.
- Choose and justify computational approach that is appropriate.
- Write the code (or add parts to MSE627-MD code)
- Perform simulations and analyze the results.
- Prepare a report/paper.
- Make a short presentation to the class (mini-symposium).

### **Timeline:**

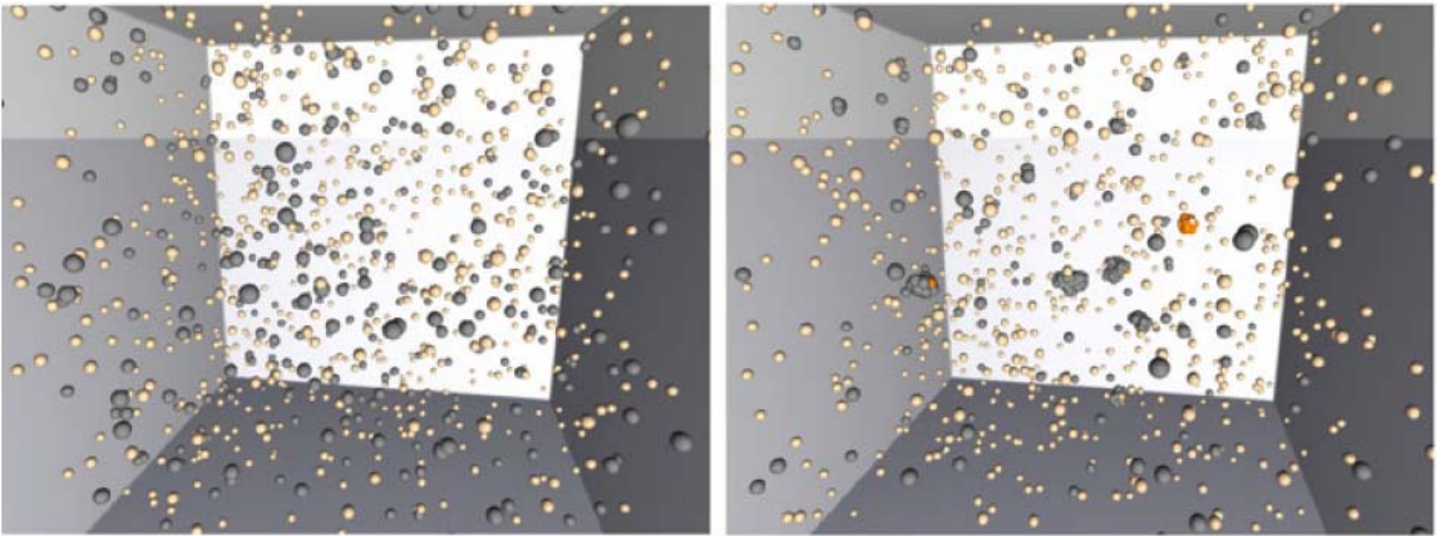
September 15 – have project approved by instructor

October 13 – turn in introduction and discuss progress with instructor

December 9 and 10 – turn in a report; present your results to the class

Below are several examples of possible term projects. **These are just examples**, you can propose your own project that is relevant to your thesis research or just seems interesting to you. If the intention is to continue computational work in the future, the term project may be a well-defined part of a larger research project.

## Cluster formation and disintegration in a vapor



N. Lümmen and T. Kraska, *Nanotechnology* **15**, 525-533 (2004)

**Research Project:** Microcanonical molecular dynamics simulation of a gaseous system with presence of clusters. Potential can be the Lennard-Jones for argon. Perform simulations for different densities and temperatures. Choose P and T based on known phase diagram for Ar. Analyze velocity distributions of atoms. Relate simulation data to Homogeneous Nucleation Theory, e. g. [F. F. Abraham, *Homogeneous Nucleation Theory* (Academic, New York, 1974)]

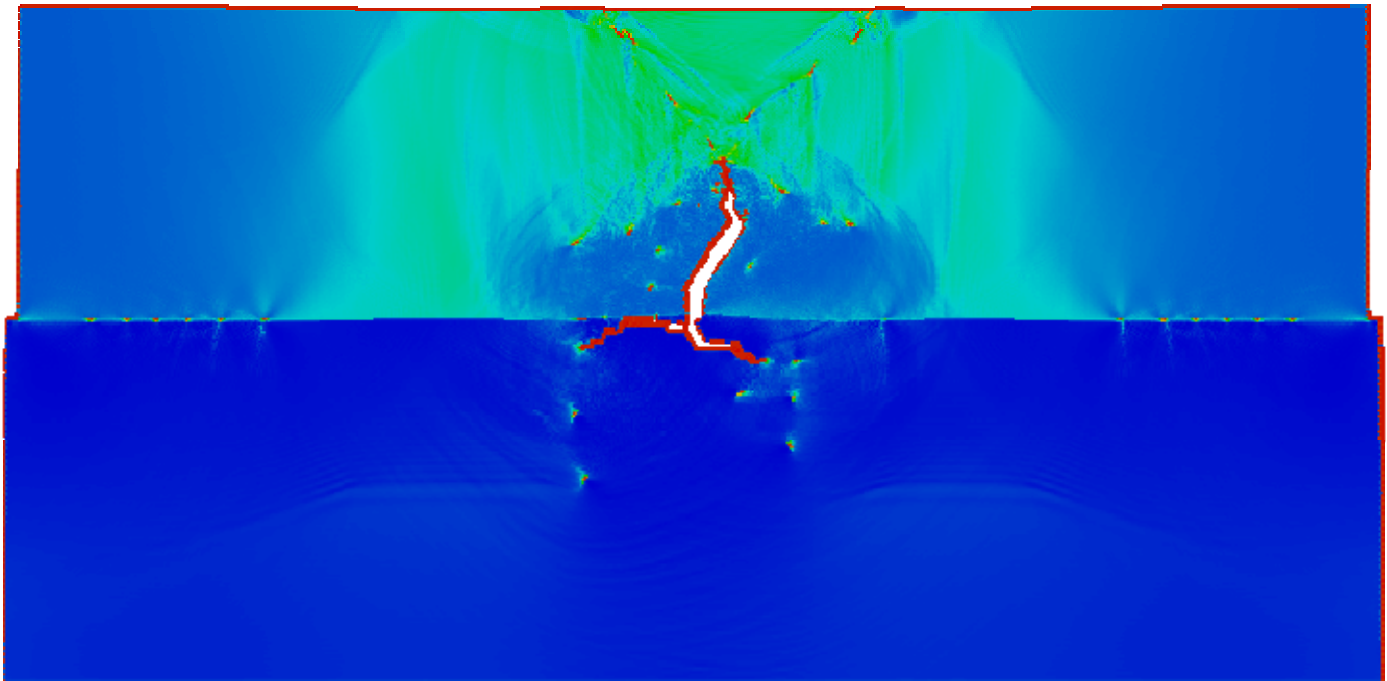
An example of MD simulation of cluster birth-death processes in a vapor:

R. Soto and P. Cordero, *J. Chem. Phys.* **110**, 7316-7325 (1999)

N. Lümmen and T. Kraska, *Nanotechnology* **15**, 525-533 (2004)

**Computational challenges:** Choosing the initial velocities of atoms based on the desired temperature; Identification of clusters; Changing volume/density; Visualization, making animations; Statistical analysis.

## Strain relief mechanisms in lattice mismatched heterostructures

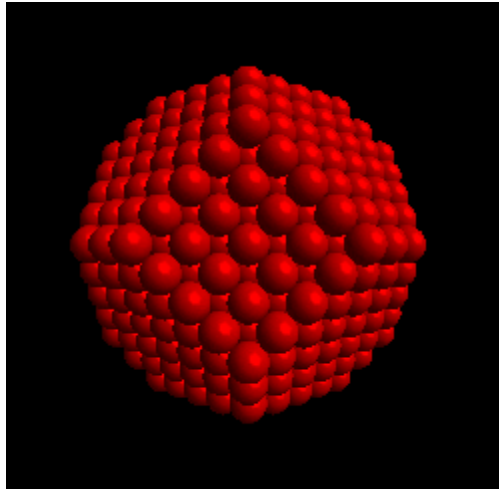


A. Kuronen, K. Kaski, L.F. Perondi, J. Rintala, *Europhysics Letters* **55** 19 (2001).

**Research Project:** Simulation of interfacial fracture due to the lattice mismatch between the overlayer and substrate. Calculate stress distributions, Analyze the mechanisms of stress relief (crack propagation, dislocation nucleation). Discuss the final defect configuration.

**Computational challenges:** Choosing parameters of Lennard-Jones potential for two lattices; Calculation of stress distribution, Structural analysis; Visualization, making animations.

## Structure of small atomic clusters



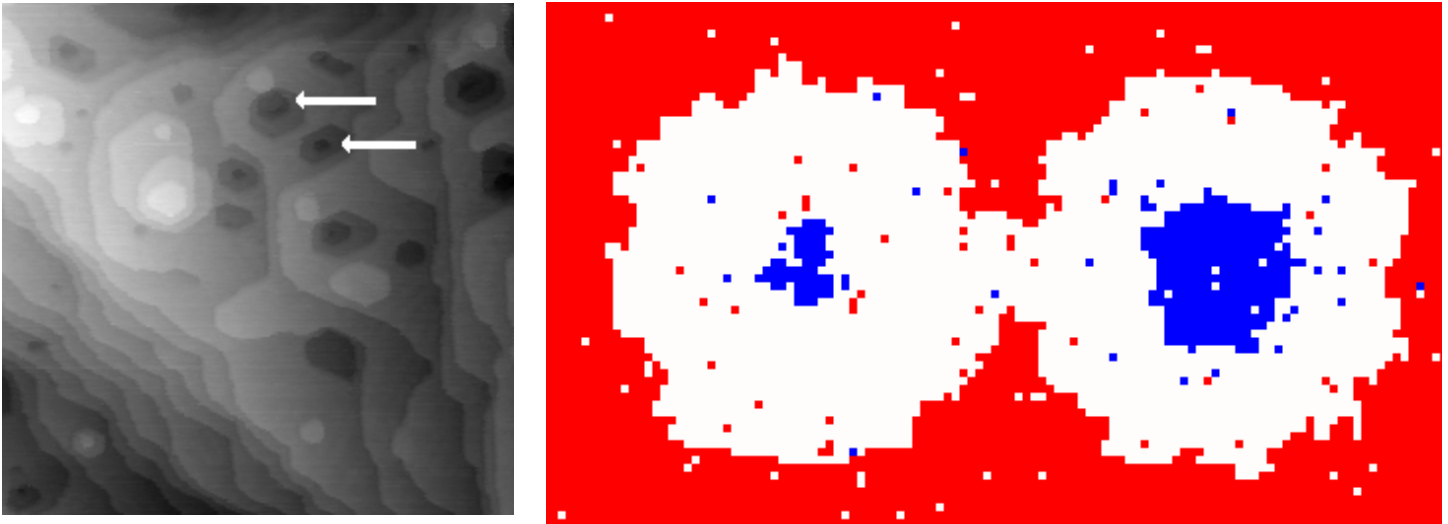
**Research Project:** Search for energetically favorable atomic configurations for small Lennard-Jones clusters of atoms. Compare non-crystalline icosahedral clusters with face-centered cubic clusters for small numbers of atoms. Which ones have lower energy? What is the role of surface and interior energies? What is the critical size when the crystalline structure becomes more stable? Compare with experimental electron diffraction data and other simulations. This study can be performed for metals as well (EAM potential).

T. Ikeshoji, G. Torchet, M. F. de Feraudy, K. Koga, Phys. Rev. E 63, 031101 (2001) - Icosahedron-fcc transition in Lennard-Jones clusters.

O. Diéguez, R. C. Longo, C. Rey, L. J. Gallego, Eur. Phys. J. D 7, 573-576 (1999) - Fe and FeAl clusters

**Computational challenges:** Making initial configurations with fcc and non-crystalline structure; Adding EAM potential in case of metal clusters; Structural analysis; Choosing and adding to the MD code an algorithm for energy minimization; Visualization.

## Stability and evolution of nanoscale features on surfaces



[http://www.lassp.cornell.edu/cooper\\_nanoscale/nanofeatures.html](http://www.lassp.cornell.edu/cooper_nanoscale/nanofeatures.html)

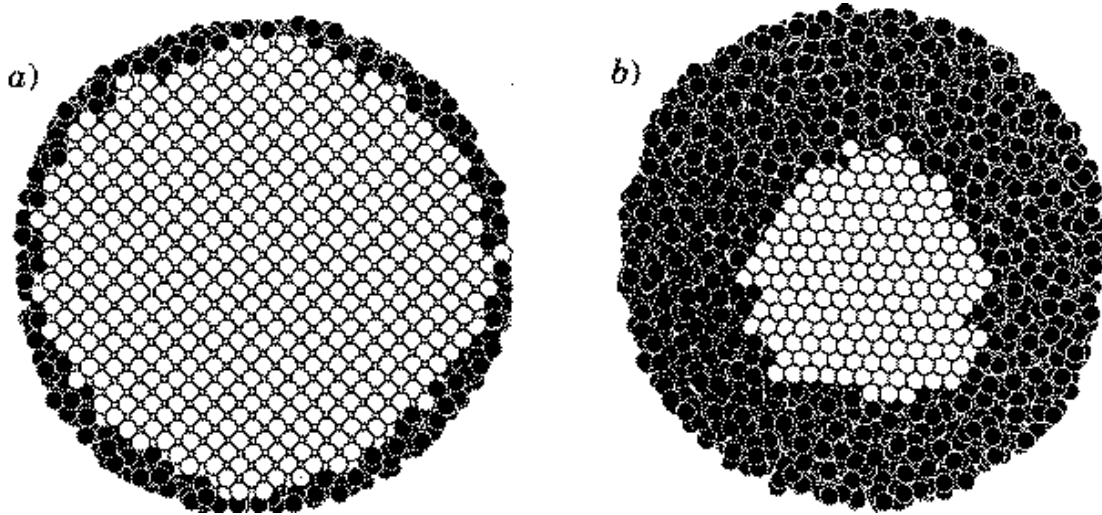
**Research Project:** Investigate the stability and evolution of nanoscale features on Si or metal surface. Modeling of the decay of islands and pits can be performed by Monte Carlo or Molecular Dynamics method. Choose a system for which experimental data is available or which is of potential technological interest. Compare simulation results with available experimental data or discuss potential implications of the results.

J. G. McLean et al., Phys. Rev. B 55, 1811 (1997)

J. G. McLean et. al., in Surface Diffusion: Atomistic and Collective Processes, ed. Michael C. Tringides, Plenum Press, New York, 1997, p. 377.

**Computational challenges:** Adding interatomic interaction potential appropriate for the system of interest to the MD/MC code; Adding/modifying algorithm for MD/MC simulation; Creating initial configuration; Visualization, making animations.

## Melting of small atomic clusters



<http://www.lassp.cornell.edu/sethna/CrystalShapes/CopperCluster.html>

**Research Project:** Simulation study of melting of small Lennard-Jones clusters. Where does melting start, how it proceeds, what are the driving forces? Is there a region of coexistence of melted surface and solid core? Is there desorption from the surface at temperatures close to the melting point? Define the onset of melting through the visual inspection and analysis of the atomic mobility. Compare with results from other simulations.

J. D. Honeycutt, H. C. Andersen, *J. Phys. Chem.* **91**, 4950-4963 (1987)

O. H. Nielsen et al., *Europhysics Lett.* **26**, 51 (1994)

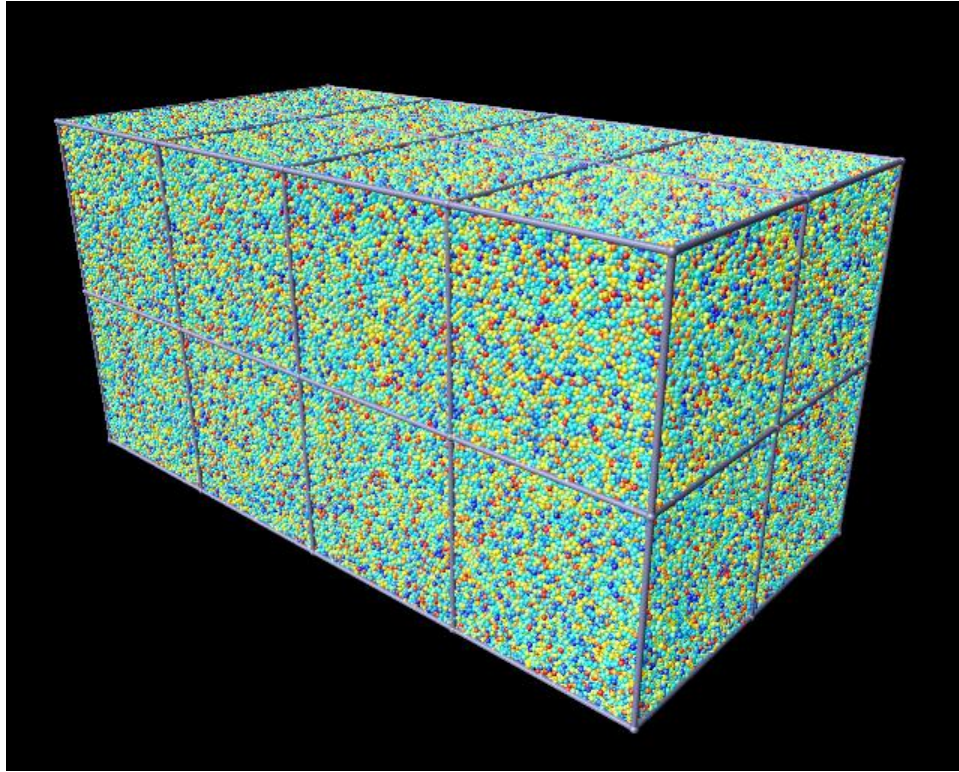
A. M. Mazzone, *Phil. Mag. Lett.* **78**, 145-152 (1998); *Phil Mag. B* **80**, 95-111 (2000)

C. L. Cleveland, W. D. Luedtke, U. Landman, *Phys. Rev. B* **60**, 5065 (1999) - Au clusters

K.-C. Fang and C.-I. Weng, *Nanotechnology* **16**, 250 (2005) - Si clusters

**Computational challenges:** Choosing the initial velocities of atoms based on the desired temperature; Performing simulations at constant energy or constant temperature conditions; Structural analysis; Visualization, making animations.

## Melting – Crystallization - Amorphization



**Research Project:** Simulation of melting, crystallization, and/or amorphization of a model material (e.g. Lennard-Jones Ar, Stillinger – Weber Si, EAM metal). Many papers have been published on this subject. A big variety of questions can be addressed.

F. Yonezawa, S. Nosé, S. Sakamoto, *Zeitschrift für Physikalische Chemie Neue Folge* **156**, 77-90 (1988) – quenching of Lennard-Jones liquid: amorphization and crystallization.

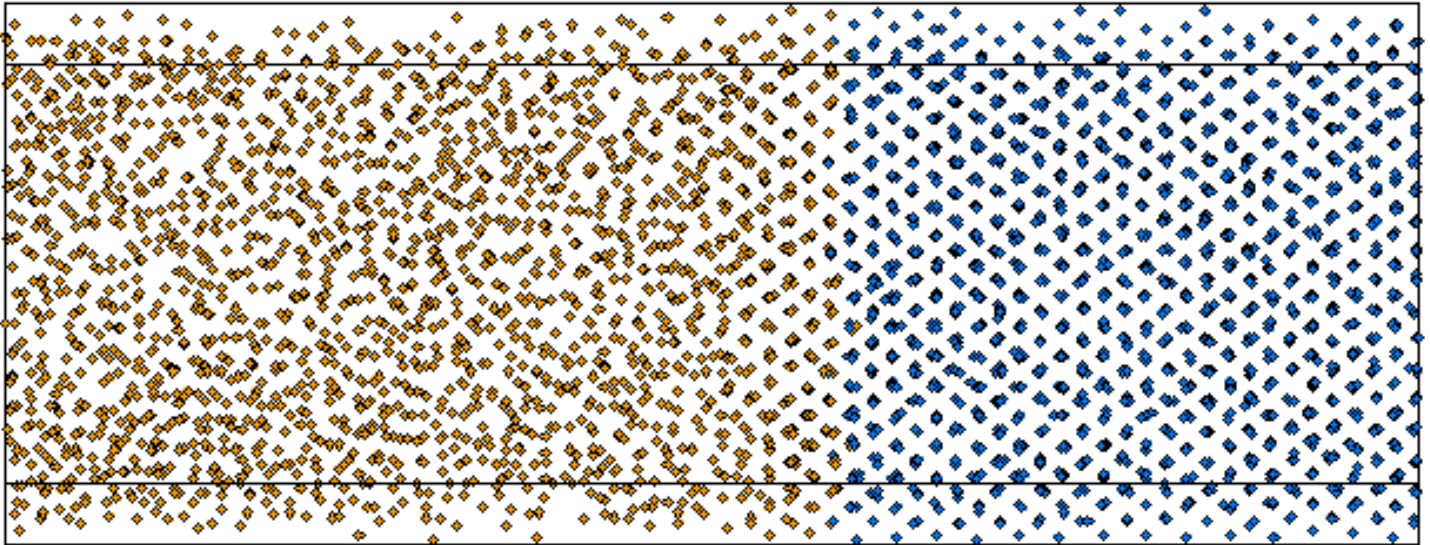
V. A. Likhachev, A. I. Mikhailin, and L. V. Zhigilei, *Phil. Mag. A* **69**, 421-436, (1994) - Quenching of nickel from the melt leading to its amorphization or crystallization.

P. R. ten Wolde, M. J. Ruiz-Montero, D. Frenkel, *J. Chem. Phys.* **104**, 9932-9947 (1996) – MD/MC simulation of crystal nucleation in a Lennard-Jones system.

F. H. Stillinger, T. A. Weber, *Phys. Rev. B* **31**, 5262-5271 (1985) – potential for Si is introduced and solid-liquid transition is explored.

**Computational challenges:** Code Nosé-Hoover constant temperature and pressure algorithm. Analysis of structural changes, dynamic properties; Visualization.

## Coexisting liquid and solid phases

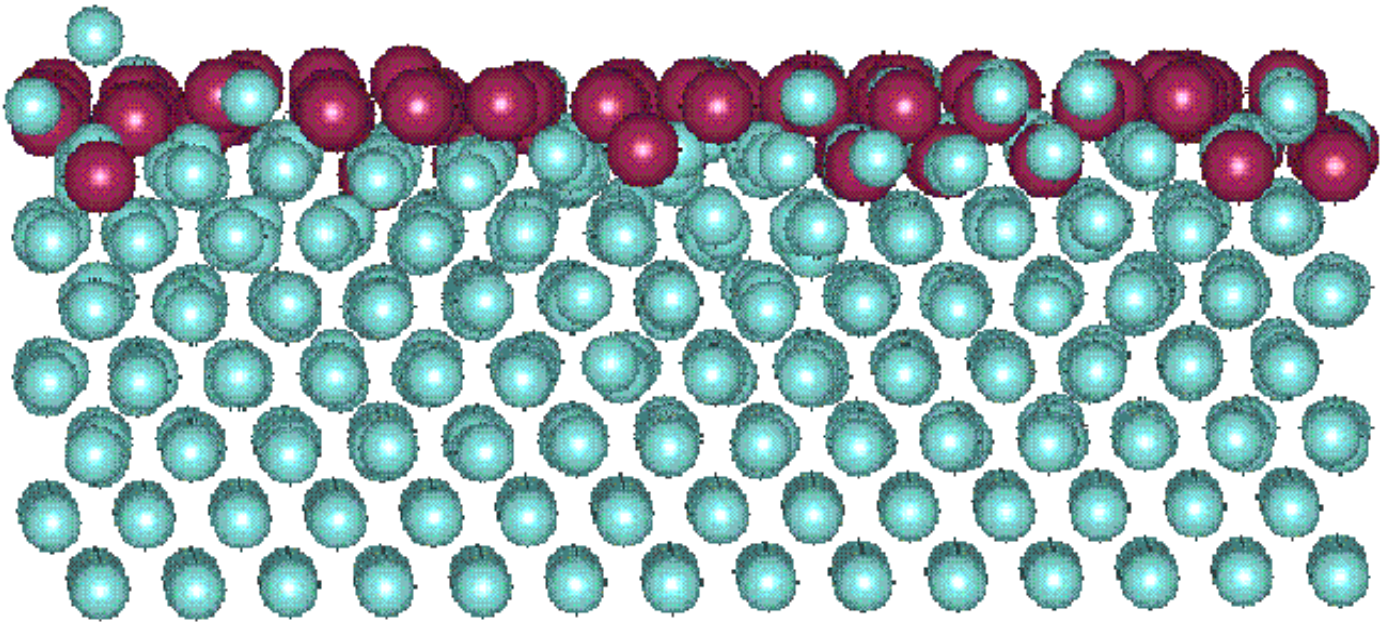


**Research Project:** Determine the melting temperature of a system (Lennard-Jones, EAM metal, Stillinger-Weber Si) by examining coexistence of a liquid and solid at a fixed pressure. Discuss various approaches that have been used to determine the melting temperature for a given potential.

J. R. Morris et al., Phys. Rev. B 49, 3109 (1994)

**Computational challenges:** Choosing appropriate boundary conditions; physics of melting and how to study it computationally; structural analysis, animations.

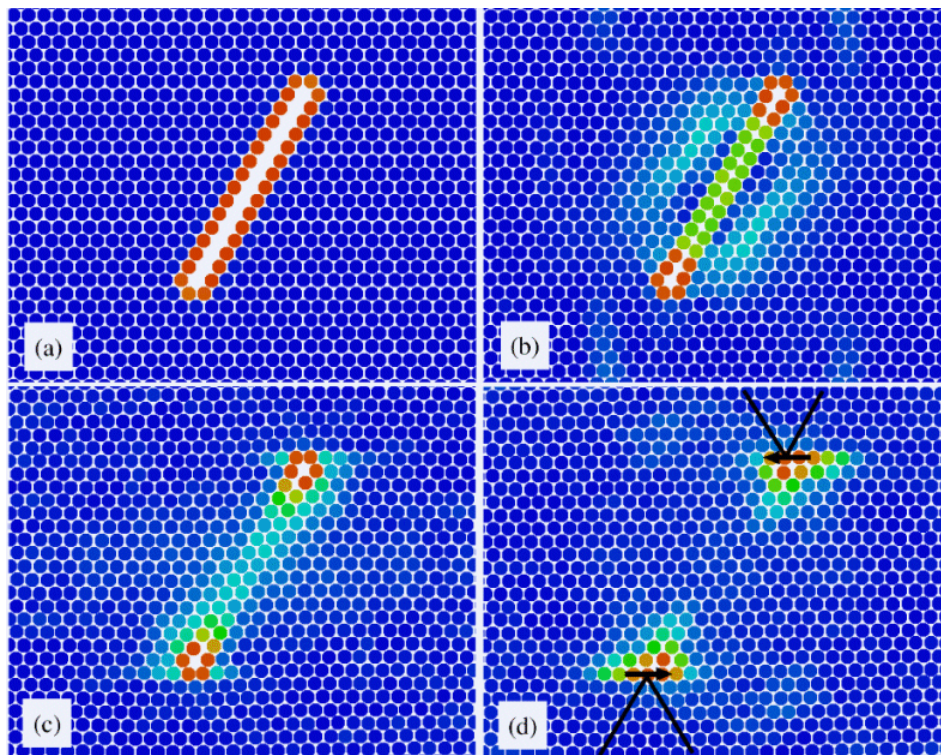
## Oscillatory surface segregation of Si-Ge alloys



**Research Project:** There is a study by P. C. Kelires & J. Tersoff, Phys. Rev. Lett. **63**, 1164-1167 (1989) in which they incorporate two kinds of Monte Carlo moves – small atomic displacements and interchange of atom type) to investigate surface segregation vs temperature in Si-Ge alloys. You can investigate similar effects for the Stillinger-Weber Si-Ge system, and/or investigate segregation of Si and Ge atoms in small clusters...

**Computational challenges:** Coding potentials; Varying types of MC moves; Making the initial atomic configuration; Choosing boundary conditions; Structural analysis; Visualization.

## Simulation of atomic structure of interfaces, dislocations, vacancies, and interstitials in two-dimensional crystals



A. Kuronen et al., University of Helsinki, Finland

**Research Project:** Simulation of atomic structures for defects and their ensembles in two-dimensional crystallites. Calculate stress distributions, compare with predictions of linear theory of elasticity. Relate simulation results to observations from experiments with soap bubbles, e. g. [A. S. Argon and L. T. Shi, *Phil. Mag. A* **46**, 275-294 (1982)].

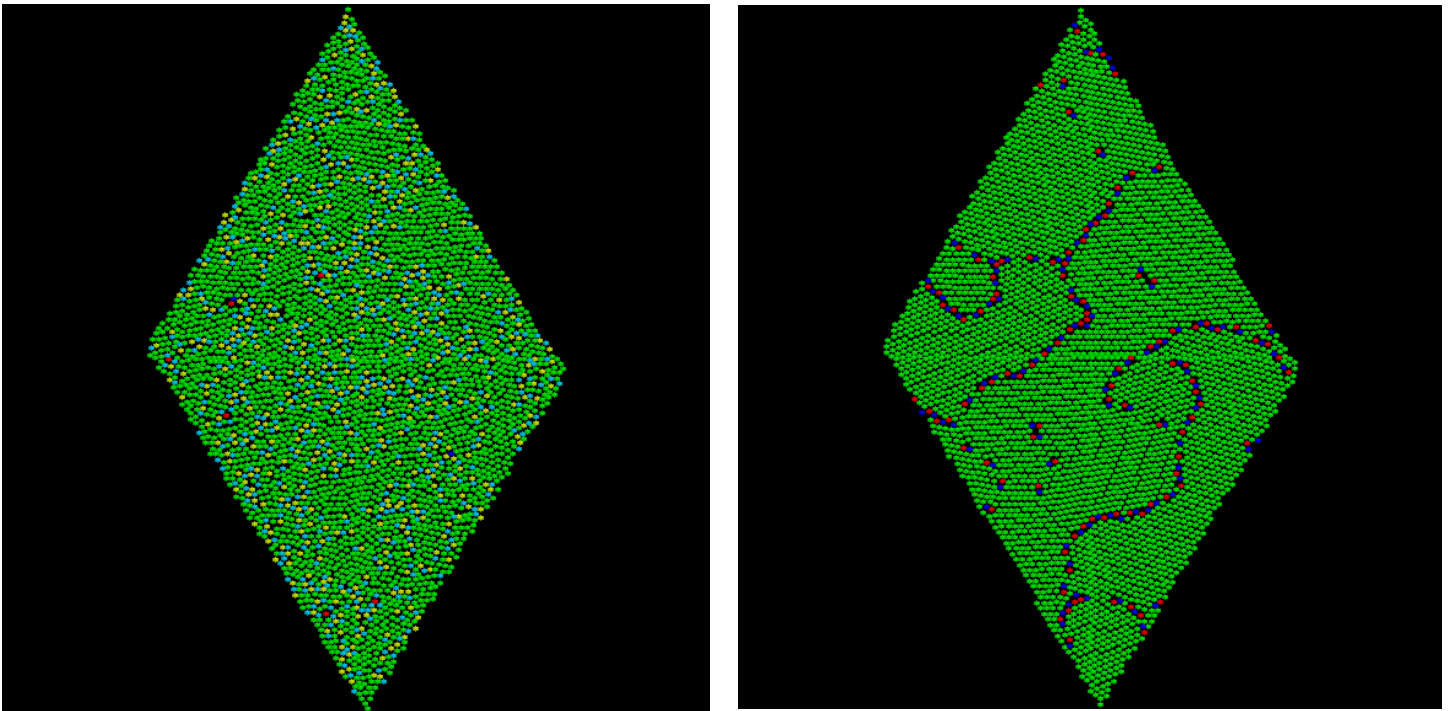
Examples of 2D MD simulations:

R. M. J. Cotterill, T. Leffers, H. Lelkolt, *Phil. Mag.* **30**, 265-275 (1974) – grain boundaries

P. O. Esbjorn and E. J. Jensen, *J. Phys. Chem. Solids* **37**, 1081-1092 (1976) – dislocations

**Computational challenges:** Making initial atomic configurations for defects; Choosing correct periodicity for grain boundaries; Structural analysis; Calculation of atomic level stresses; Visualization, making animations.

## Simulation of dynamic processes in two-dimensional crystals



F.L. Somer et al., Phys. Rev. Lett. 79, 3431 (1997); Phys. Rev. E 58, 5748 (1998)

**Research Project A.** Test a theory for melting in two dimensions that was developed by Kosterlitz, Thouless, Halperin, Nelson, and Young (the KTHNY theory, after the initials of its authors' last names).

<http://www.ornl.gov/ORNLReview/v30n3-4/solids.htm>

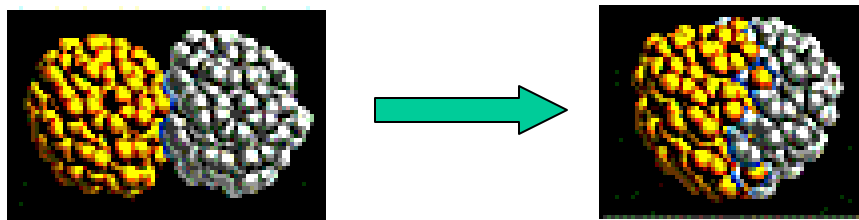
<http://www.csm.ornl.gov/~tsk/meltingsum.html>

**B.** Study generation of a dislocation cloud screening the elastic field of a disclination introduced into a finite-size crystallite.

A. E. Romanov, Materials Science and Engineering A **164**, 58-68 (1993)

**Computational challenges:** Preparing initial atomic configurations; Analysis of structural changes; Calculation of atomic level stresses; Visualization, making animations.

## Collision of small atomic clusters



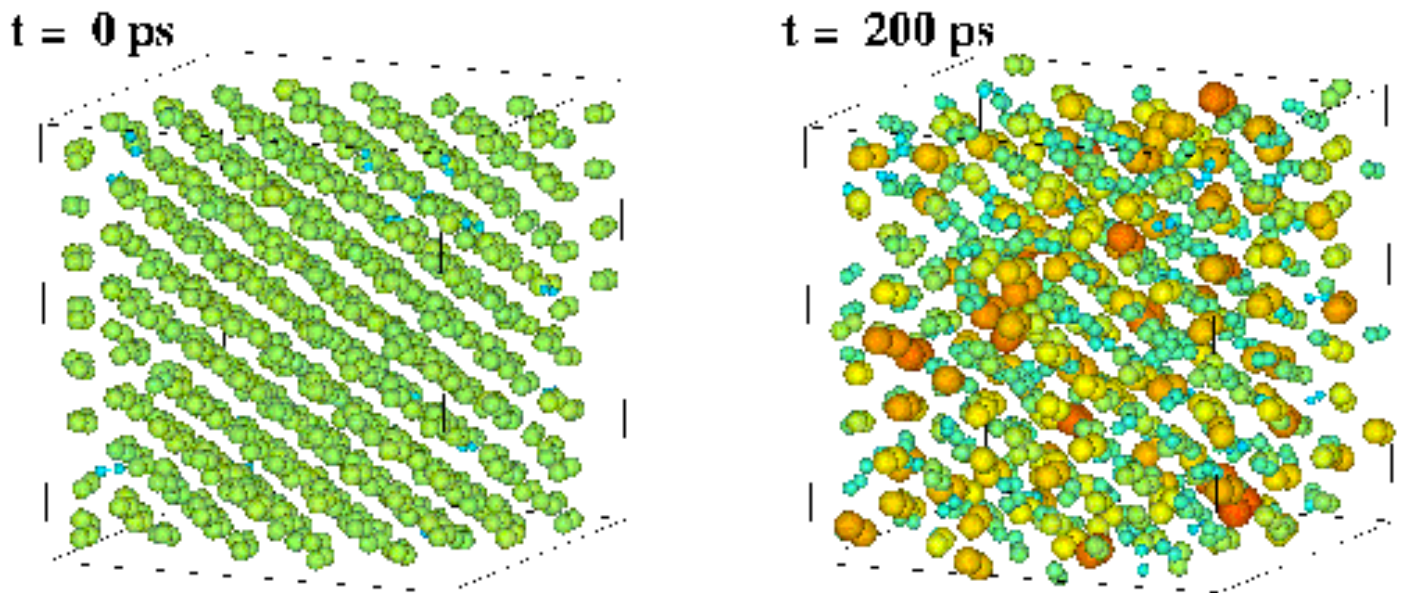
<http://www.csi.gmu.edu/lcdm/pub/p4.html> - link is not active

**Research Project:** Simulation study of the dynamics of colliding clusters, study the development of temperature, potential energy, transformation of the shape of the resulting particle. What are the energy transformations during the collision? What is driving the subsequent reshaping of the resulting particle? Is temperature increasing or decreasing in this processes?

An example for silicon nanoparticles: M. R. Zachariah, M. J. Carrier, and E. Blaisten-Barojas, *J. Phys. Chem.* **100**, 14856-14864 (1996)

**Computational challenges:** Choosing the initial velocities of atoms; Quantitative analysis should be inspired by structural analysis, visualization, and animations.

## Vibrational energy transfer and phase transformations in solid/liquid O<sub>2</sub>

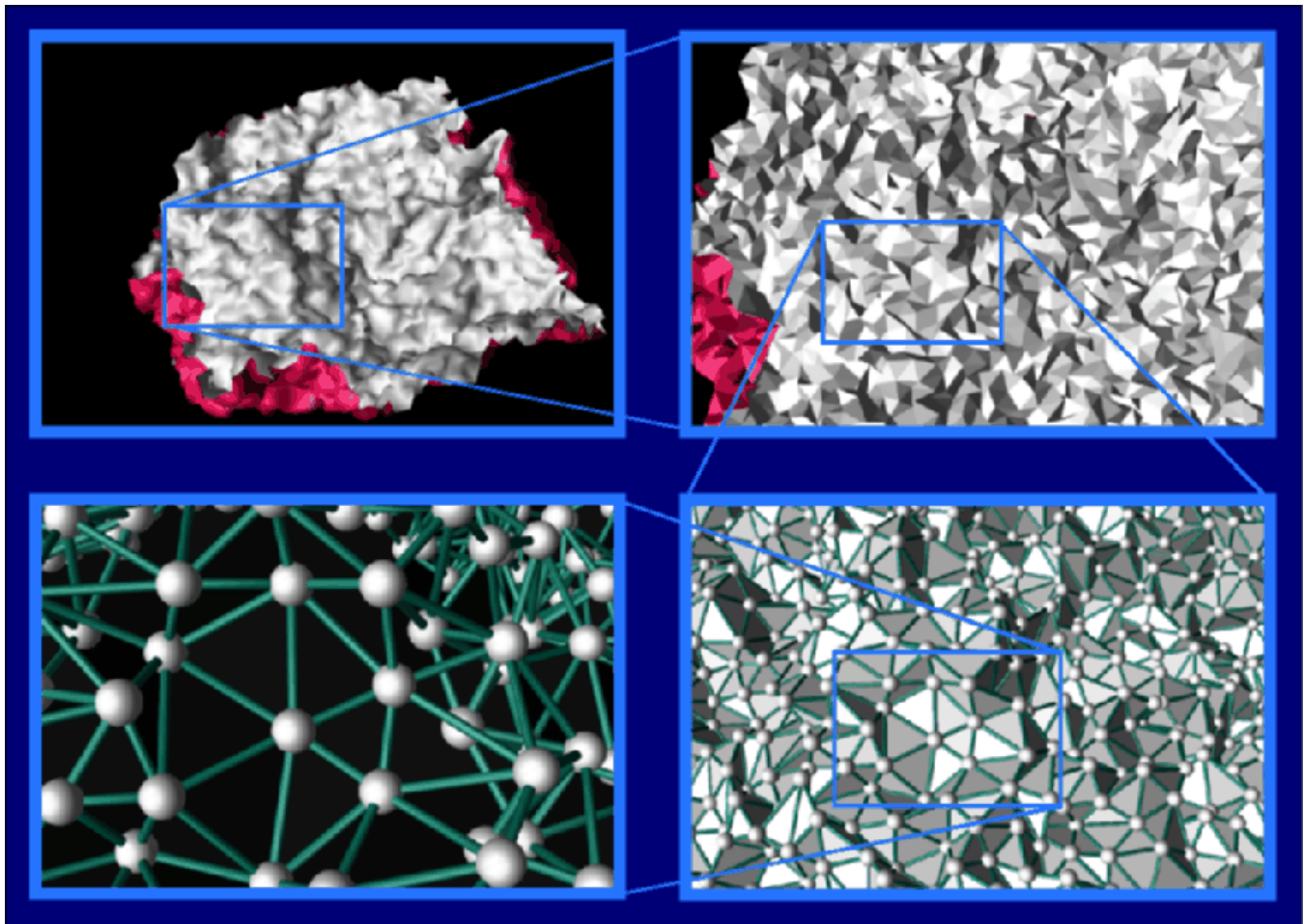


Ł. Dutkiewicz et al., J. Phys. Chem. A **103**, 2925-2933 (1999).

**Research Project:** Simulation of solid oxygen. Study the transfer of vibrational energy into lattice motion. What is the dependence of the rate of the energy transfer from the parameters of interatomic potential? How the parameters of the potential are related to the frequencies of molecular vibrations? Relate the results to the observations by Ł. Dutkiewicz et al., J. Phys. Chem. A **103**, 2925-2933 (1999).

**Computational challenges:** Making the initial atomic configuration for solid O<sub>2</sub>; Changing interatomic potentials; Adding multiple timestep integration into the MD code; Calculation of characteristic frequencies of atomic vibrations; Visualization.

## The Tethered Membrane - a Model of Random Surface

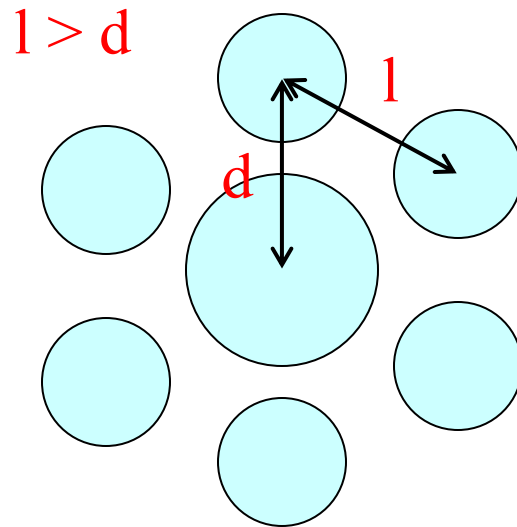


**Research Project:** A simple model of polymerized membranes, the tethered membrane, has been proposed as a model to study the large-scale properties of random surfaces (microemulsions, lipid bilayers, vesicles, and suspensions of monolayers of exfoliated layered crystals). You can reproduce some of the results of this study and extend the model to address new questions. This project is especially suitable for a physicist.

Description of the results and references can be found at <http://www.almaden.ibm.com/vis/membrane/overview.html>

**Computational challenges:** Development (based on MSE627-MD) of a computer code for the tethered membrane model; Temperature control; Structural analysis; Visualization, making animations.

## Molecular dynamics on a surface of constant curvature



Seven particles of the same size arranged in a hexagon in a curved space

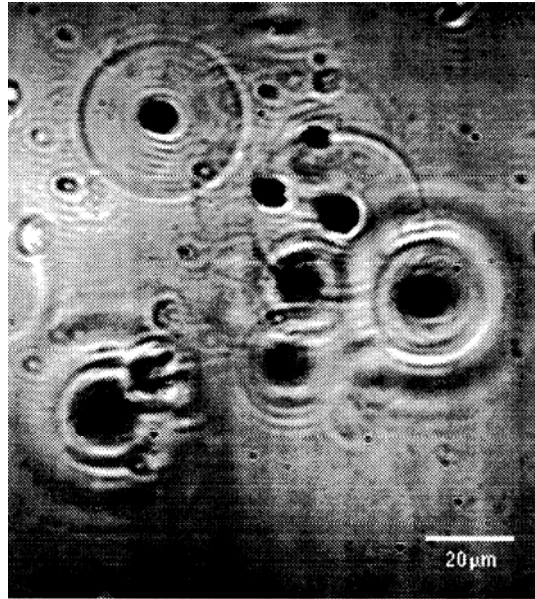
**Research Project:** Modify molecular dynamics algorithm for a two-dimensional space of constant curvature. Perform simulations of a close-packed system in the curved space. What is the structure? Why? This project is especially suitable for a physicist with a taste for mathematics.

D. R. Nelson, Phys. Rev. B. **28**, 5515-5535 (1983); Solid State Physics **42** (1989).

J. P. Straley, Phys. Rev. B. **30**, 6592-6595 (1984).

**Computational challenges:** Modification of molecular dynamics code to reproduce a curved space; Structural analysis of a two-dimensional system; Visualization, making animations.

## Explosive boiling of liquid adjacent to a heated surface



C. P. Lin, M. W. Kelly, in *Laser-Tissue Interaction VIII*, SPIE, **2975**, 174-9 (1997)

**Research Project:** Laser heating of a surface adjacent to a fluid causes bubble formation, as pictorially demonstrated in high-speed imaging experiments of melanosomes irradiated by a 30 ps laser pulse (picture above). But what is the mechanism of bubble formation? In general, what is the mechanism of energy transfer through the interface separating materials with drastically different thermal properties?

C. P. Lin, M. W. Kelly, *Appl. Phys. Lett.* **72**, 2800-2802 (1998) – experiment for irradiated melanin particles in water.

S. Merabia, P. Keblinski, L. Joly, L. J. Lewis, J. L. Barrat, *Phys. Rev. E* **79**, 021404 (2009) – MD simulation of heated nanoparticle surrounded by fluid.

**Computational challenges:** Developing a 2D or 3D model of two-component system; Developing boundary conditions for non-reflecting propagation of the laser induced pressure wave from the MD computational cell; Visualization.