Computational Physics

Project: Molecular Dynamics

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Introduction

In this report, we use molecular dynamics (MD) simulations with empirical atomic potentials, focusing on germanium (Ge). Empirical potentials, such as Lennard-Jones and Stillinger-Weber, are simplified models that represent atoms as classical particles. They neglect the quantum mechanical properties of electrons and provide an efficient way to simulate atomic interactions.

Task 1: Lattice constants, Cohesive Energies, and Bulk Modulus

We use the Stillinger-Weber (SW) potential, which includes two- and three-body interactions, to study the behavior of Ge atoms in various crystal structures. We have four different crystal structures: diamond, face-centered cubic (fcc), body-centered cubic (bcc), and simple cubic (sc).

For each structure, we followed these steps:

1. We created larger supercells with different lattice constants using `crystals.ipynb`.

2. We ran simulations via LAMMPS to compute the total energy for each lattice constant value.

3. We applied the Murnaghan equation of state fit via `murnaghanFit.ipynb` to find the energetically favorable structure.

We present the Murnaghan fits for the different structures:
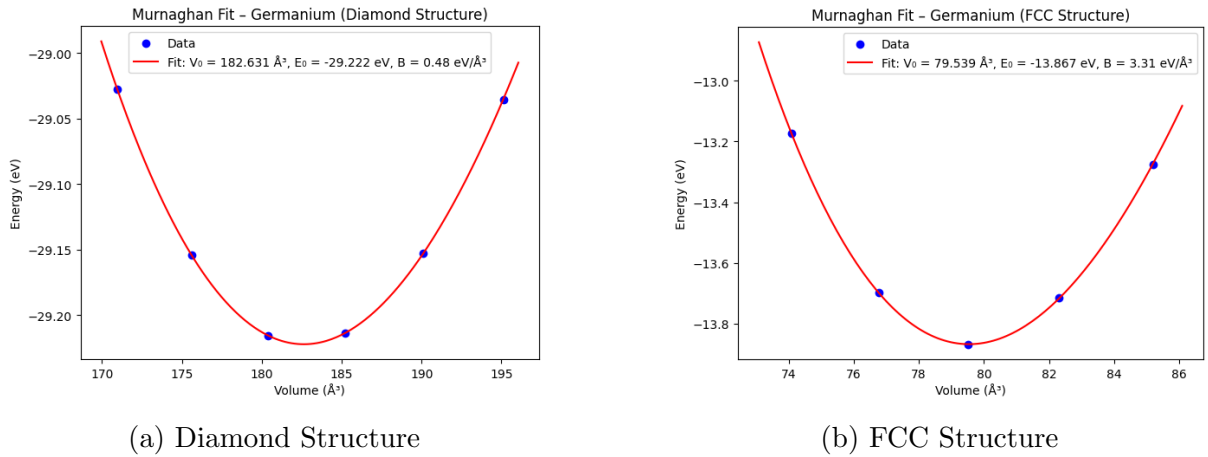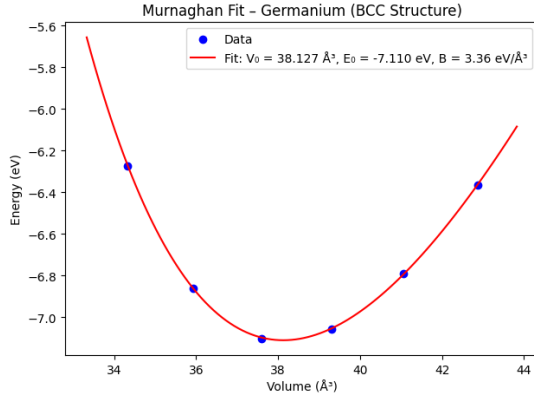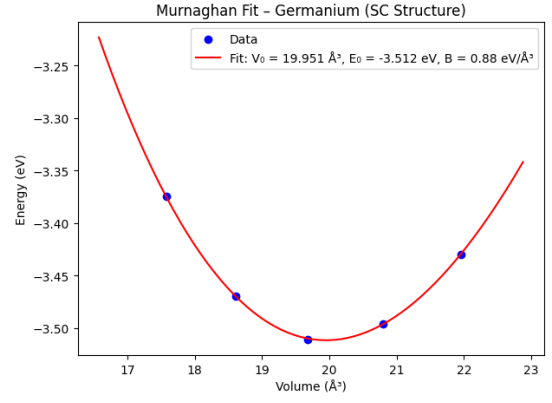

| (a) Diamond Structure | (b) FCC Structure |

Figure 1: Ge structures in four different crystal arrangements.

(a) BCC Structure   (b) SC Structure

Figure 2: Ge structures in four different crystal arrangements.

The basic material properties such as lattice constants, cohesive energy, bulk modulus, and others for the different crystal structures are listed in the tables below:

Table 1: Ge Characteristics

Structure	A (Å)	V (Å^3)	Cohesive Energy (eV)
Diamond	5.673614235	182.6330663	-3.652772726
FCC	4.300583521	79.53937231	-3.466849802
BCC	3.365724719	38.12727589	-3.554815215
SC	2.712185042	19.95069133	-3.511797022

Table 2: Ge Characteristics

Structure	Total Energy (eV)	B (eV/Å^3)	B (GPa)
Diamond	-29.22218181	0.477569676	76.51509692
FCC	-13.86739921	3.305204145	529.5520809
BCC	-7.109630429	3.36308986	538.8263948
SC	-3.511797022	0.879290216	140.8778227

(Where: 1 eV/Å^3 = 160.21766208 GPa)

Comment: The very high bulk modulus values, even exceeding 500 GPa, are reasonable as we are examining metastable phases. We have packed the atoms in these structures in physically unnatural geometries. However, the tetrahedral geometry of the diamond structure allows easier compression.

In conclusion, the diamond structure exhibits the lowest cohesive energy, indicating that it is the most stable among the others due to the directional covalent bonds and compatibility with the electronic structure. This result was expected.

Task 2: Melting Temperature

In this part of the report, we perform MD simulations to investigate the thermal behavior of Ge, specifically its melting point. We then analyze atomic arrangements and pair correlation functions as temperature increases.

A supercell of 216 atoms was used with the file `in.mel.lammps`, where for each temperature T we ran MD simulations with 2×10^5 timesteps (with $t_{\text{step}} = 0.001$ ps). The temperature was varied gradually.

For each temperature, the following were recorded:

- Kinetic energy (K)

- Potential energy (P)

- Temperature (T)

from the file `energy.dat`, keeping the last line, which includes the average values over the last 10^5 steps. Presenting the results, we observe:
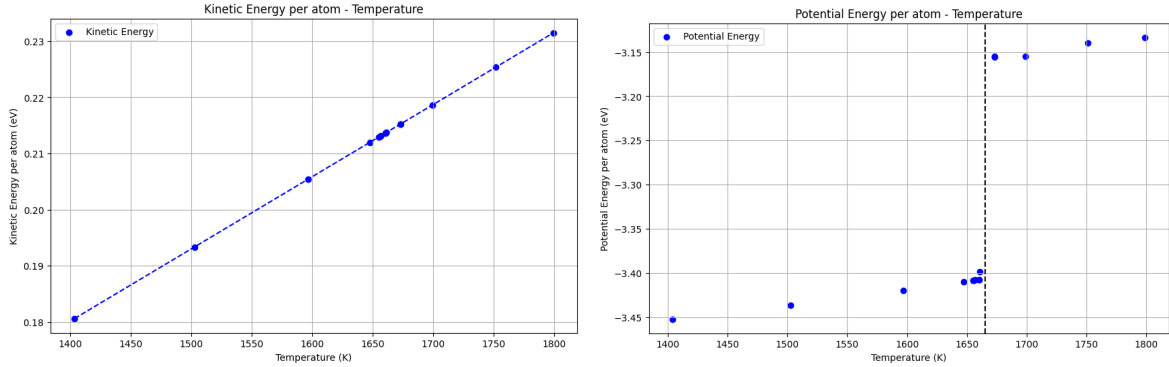

Figure 3: Left: Kinetic energy vs Temperature. Right: Potential energy vs Temperature.

The potential energy (P) shows a sharp change around $T \approx 1650$–1660 K. This sudden increase is indicative of melting, as the system transitions from the crystalline to the liquid phase. This value does not correspond to latent heat but to the temperature at which the phase transition occurs.

Next, we analyzed snapshots of atomic arrangements and pair correlation functions at temperatures 0 K, 1600 K, and 1750 K. We observe the transition from crystalline order to amorphous or liquid states as temperature increases. The files `dump.200000` for $T = 1600$ K and $T = 1750$ K were used for visualization in Ovito.

The observations were:

- At $T = 0$ K: The function shows high and sharp peaks, indicative of the long-range order of a well-organized crystal lattice, where the distances between neighboring atoms are well defined. The first peak of $g(r)$ corresponds to the nearest neighbor distance.

- At $T = 1600$ K: There is a slight decrease in peak height and an increase in peak width, indicating thermal disturbances but no loss of crystallinity yet.
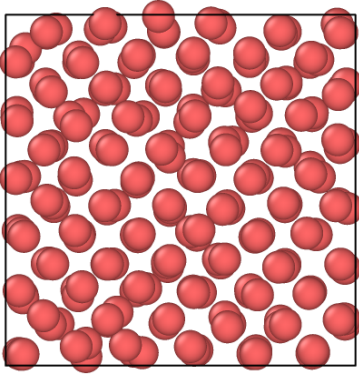
- At $T = 1750$ K: The structure loses long-range order, while the peaks in $g(r)$ become broader and less pronounced, characteristic of the liquid phase.
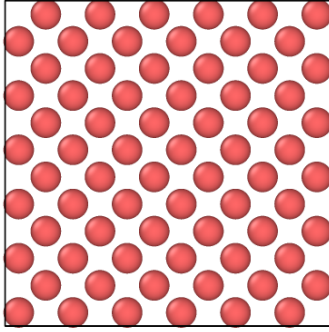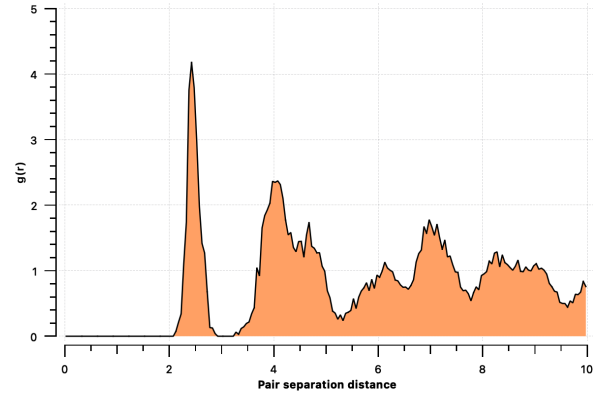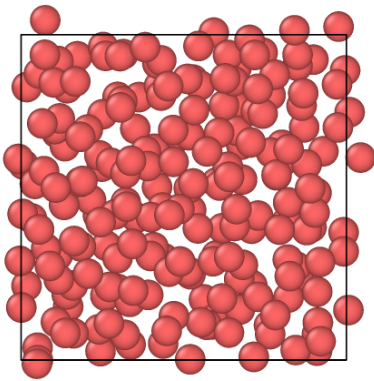

(a) Structure at $T = 0$ K
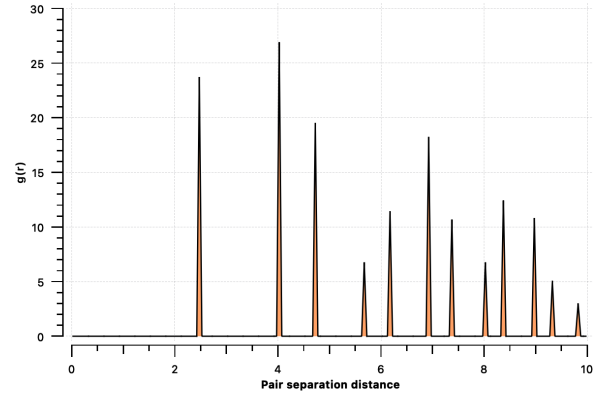
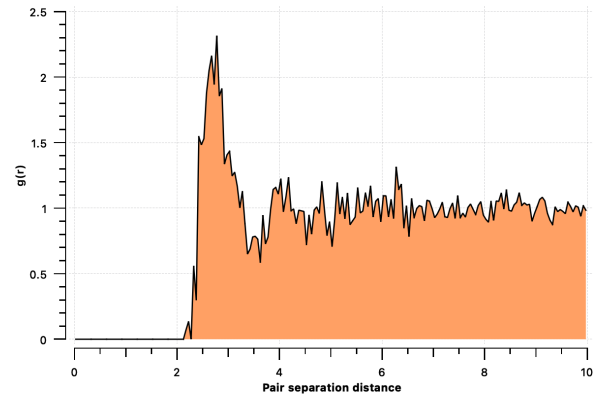(b) Pair correlation function $g(r)$ at $T = 0$ K

(c) Structure at $T = 1600$ K

(d) Pair correlation function $g(r)$ at $T = 1600$ K

(e) Structure at $T = 1750$ K

(f) Pair correlation function $g(r)$ at $T = 1750$ K

Figure 4: Evolution of the structure and pair correlation function $g(r)$ at different temperatures.

Comparing the $g(r)$ functions at different temperatures, we observe the microscopic reorganization of the system.

Conclusions

From the study of Ge structures, we understood that the diamond structure has the lowest cohesive energy, indicating that it is the most stable structure. Moreover, the sharp change in potential energy, combined with the observed loss of crystalline order with increasing temperature, indicate that the melting temperature of Ge, according to the empirical Stillinger-Weber potential, is around 1650 K.