Simulation of thermal expansion in silver using LAMMPS

Kamil Eliaszuk and Martyna Jankowska

ABSTRACT

Computer simulations are useful tools for modelling and studying various physical processes. Especially when the conditions cannot be easily applied in real life. In our work we used molecular dynamics simulation method to observe thermal expansion in solid silver and compute its linear and volume expansion coefficients. The simulation was run in LAMMPS, visualizations were made using OVITO and the data analysis was made in Python.

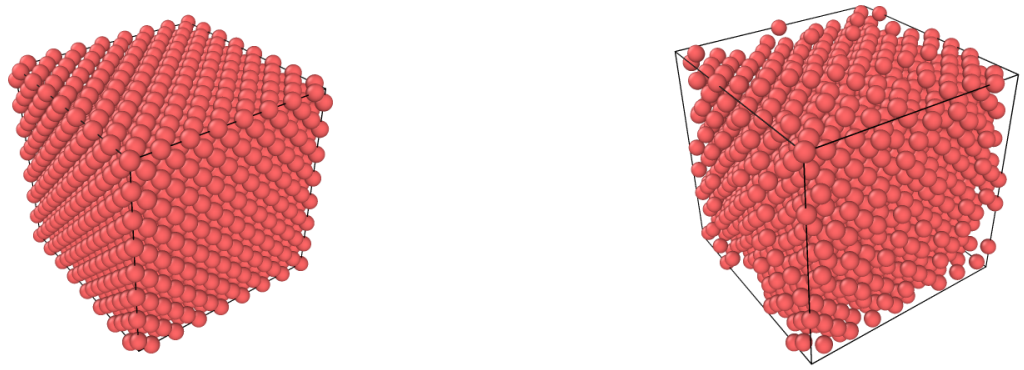
Introduction

Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) is a molecular dynamics program that can be used for modelling atoms and materials. For our simulation we chose a single metallic element - silver. It has a face-centered cubic (fcc) crystal structure and remains in the solid state throughout the simulation (from 300K to 400K). The structure consisted of 8 X 8 X 8 unit cells with a total of 2048 atoms. At the start of the simulation (200000 steps) the temperature was kept constant so that the atoms could move randomly for some time. This way pressure and volume could resemble more real-world conditions. Then the structure was heated linearly from 300K to 400K (500000 steps). The lenght of each step was 1 fs.

Results

Structure visualization

To visualize the structure we used OVITO - Open Visualization Tool for inspecting particle-based simulations. In Fig.1 there are shown two simulation frames - first of the ideally generated structure (a) and second right before the heating



(a) Ideal structure **(b)** Structure before heating

Figure 1. After 200000 steps the structure looked a lot more realistic, had different volume and pressure

Then the heating started but the changes of volume were too small to be seen on frames.

Linear expansion

Linear-expansion coefficient is defined as:

$$\alpha = \frac{1}{L}\frac{dL}{dT} \tag{1}$$

where L is a particular length measurement and $\frac{dL}{dT}$ is the rate of change of that linear dimension per unit change in temperature.

The simulation provided a set of measurements of volume in the function of temperature (where lenght can be calculated as the cube root of volume). We can create a linear regression to that set and the slope of it will be equal to $\frac{dL}{dT}$. The chart with measurements and linear regression is shown in Fig.2

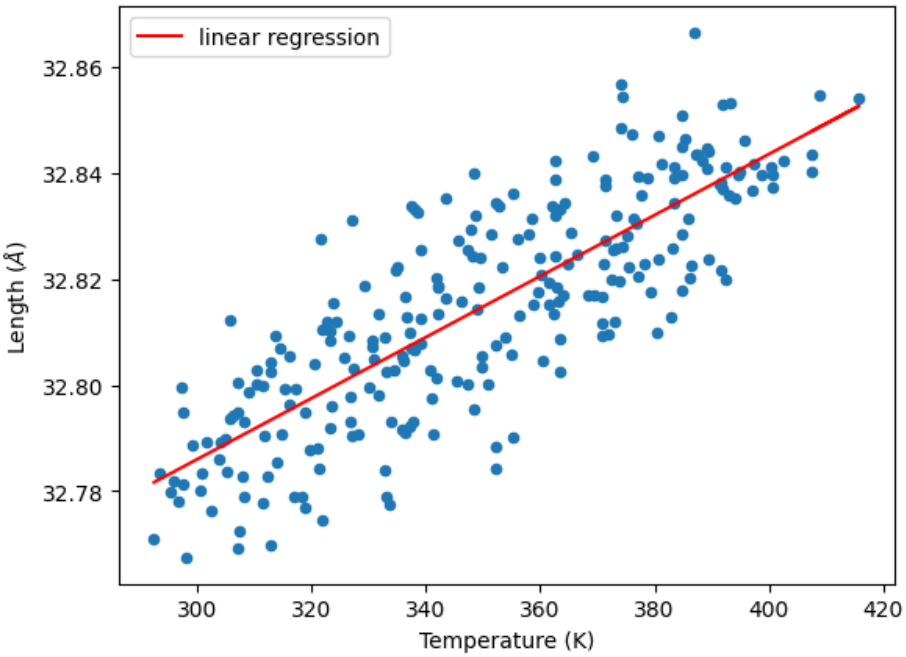


Figure 2. Lenght in the function of temperature

Having the slope value we can calculate the linear-expansion coefficient

$$\alpha = 1.765 \cdot 10^{-5} \frac{1}{K} \tag{2}$$

Volume expansion

Volumetric-expansion coefficient can be written as:

$$\beta = \frac{1}{V} \frac{dV}{dT} \tag{3}$$

where V is the volume of the material, and $\frac{dV}{dT}$ is the rate of change of that volume with temperature.

In the same way as we did with linear expansion, we can create a linear regression to the set of volume measurements and calculate its slope. The chart with measurements and linear regression is shown in Fig.3

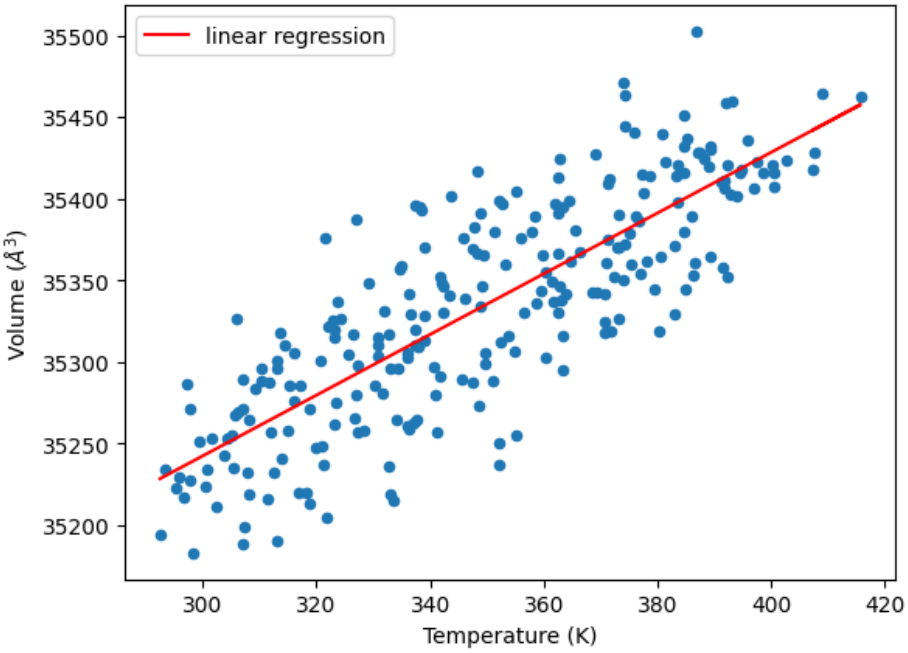


Figure 3. Volume in the function of temperature

Likewise, we can calculate the volumetric-expansion coefficient

$$\beta = 5.360 \cdot 10^{-5} \frac{1}{K} \tag{4}$$

Discussion

Both lenght and volume should be linear functions of temperature. Our measurements were not extremely precise (probably due to relatively small scale of the structure) but they had an noticeable linear tendency. As to coefficients, the results were close to literature data. For silver in 300K the values of coefficients are approximately: $\alpha = 1.9 \cdot 10^{-5} \frac{1}{K}$ and $\beta = 5.8 \cdot 10^{-5} \frac{1}{K}$

Methods

Modified embedded-atom method (MEAM)

To simulate the interactions between atoms we used modified embedded-atom method. Embedded atom model is an approximation describing the energy between atoms and is a type of interatomic potential. The energy is a function of a sum of functions of the separation between an atom and its neighbors. The modified embedded atom method (MEAM) is an empirical extension of the embedded atom method that includes angular forces.

References

1. B.-J. Lee, J.-H. Shim, and M.I. Baskes (2003), "Semiempirical atomic potentials for the fcc metals Cu, Ag, Au, Ni, Pd, Pt, Al, and Pb based on first and second nearest-neighbor modified embedded atom method", Physical Review B, 68(14), 144112. DOI: 10.1103/physrevb.68.144112.

2. Aidan P. Thompson, H. Metin Aktulga, Richard Berger, Dan S. Bolintineanu, W. Michael Brown, Paul S. Crozier, Pieter J. in 't Veld, Axel Kohlmeyer, Stan G. Moore, Trung Dac Nguyen, Ray Shan, Mark J. Stevens, Julien Tranchida, Christian Trott, Steven J. Plimpton, LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales, Computer Physics Communications, Volume 271, 2022, 108171, ISSN 0010-4655, https://doi.org/10.1016/j.cpc.2021.108171.