Title of the master thesis

by

Filip Henrik Larsen

Thesis

for the degree of

Master of Science

Faculty of Mathematics and Natural Sciences
University of Oslo

May 2017

Abstract

This is an abstract text.

To someone

This is a dedication to my cat.

Acknowledgements

Flora Joelle Larsen
Anders Hafreager

Contents

Chapter 1

Introduction

Why is the subject of this thesis of any interest?
What is our take on the problem?
What do we hope to accomplish?
How will this be of any contribution to anything?
How is the thesis laid out?

Chapter 2

Setting up the system

We wish to construct a system consisting of two elements made out of silica: a slab and a sphere cap. In order to do this we need to generate the spacial position coordinates (x,y,z) of every single atom. Considering that we are making a system consisting of about 10^5 atoms, this is obviously not done manually. We have chosen to use a tool named *Moltemplate*[1], which is included in the LAMMPS distribution.

The main idea is to manually enter the coordinates of only the atoms in a unit cell of the material one wish to generate, and then simply copy this unit cell wherever desired. The software will shift the coordinates of the copied unit cell by the displacement from the original image. In addition it will generate files containing data such as which atoms they share bonds with, if any, and angles between such bonds.

2.1 Silica

Silica is a chemical compound also known as Silicon dioxide, having the chemical formula SiO_2. It has several polymorph structures, the most common being quartz, which is one of the most abundant minerals in the Earth's crust. Other polymorphs include cristobalite, tridymite, coesite and more. In this project we will build the constituents of the system from a variety named β-cristobailte. This is mainly because it has a simple structure and a cubical unit cell. The length of each edge is 7.12Å.

2.1.1 Unit cell of β-cristobalite

In order to construct the unit cell of a material, one should look up the coordinates of the atoms in a crystallography database. We have used the unit cell

[1] http://www.moltemplate.org/index.html

of β-cristobalite found at *Crystallography Open Database*[2]. At this site one can download a `.cif`-file consisting of the spatial positions of each atom, the length of the unit cell edges, and the angles between the faces of the cell. In the case of β-cristobalite the unit cell is cubical with sides of length 7.12Å. It contain 8 silicon atoms and 16 oxygen atoms. The density of the unit cell can easily be computed and is 2.2114 g/cm^3.

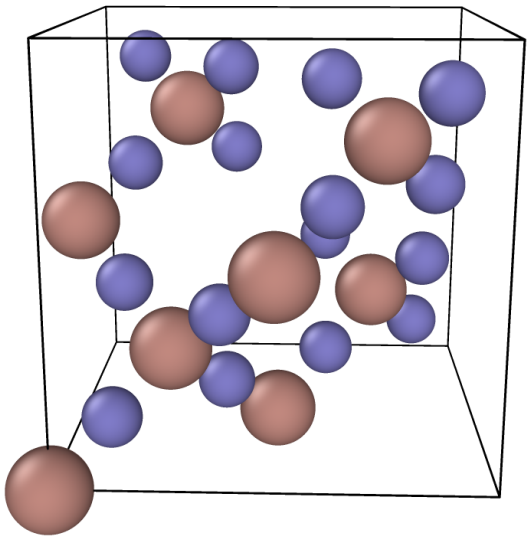

Figure 2.1: Unit cell of b-cristobalite. One of the easiest unit cells of the silica variations, due to the cubical structure and few atoms.

[2] http://www.crystallography.net/cod/1010944.html

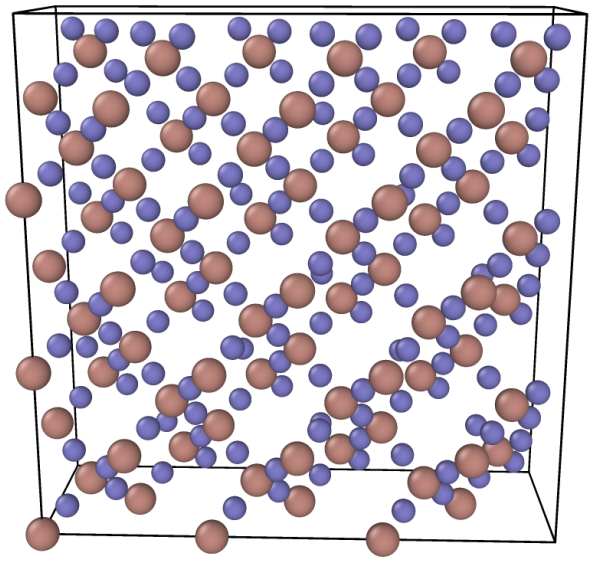

Figure 2.2: Unit cell of b-cristobalite. One of the easiest unit cells of the silica variations, due to the cubical structure and few atoms.

2.1.2 Shaping the system

The coordinates gotten from the `.cif`-file can now be implemented into *moltemplate* together with data of whatever bond and angle data required. In this case, we will use the Vashishta potential, which does not require these. We use the unit cell as building blocks, placing them concurrently until we have a crystal of the desired size. For our purpose, we generate a large cube of $15 \times 15 \times 15$ unit cells, as shown in Figure 2.3. This system contain 81000 atoms.

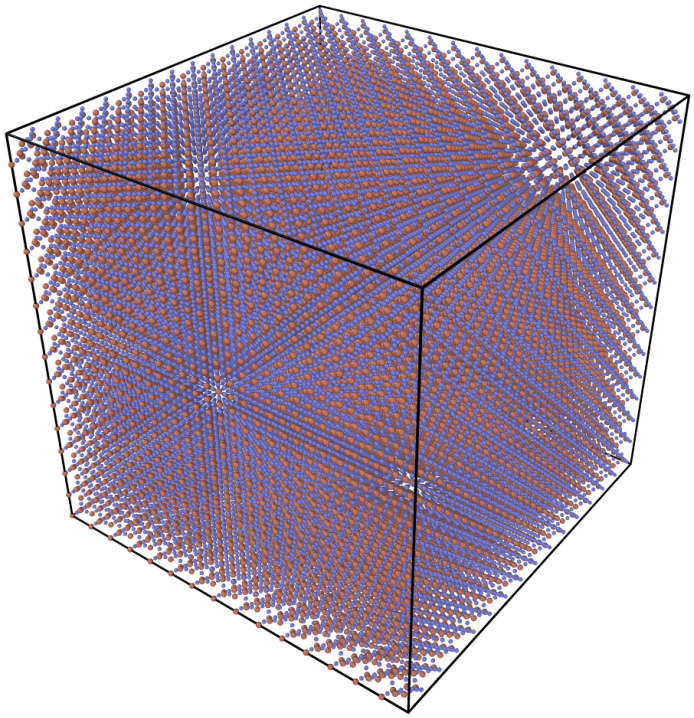

Figure 2.3: System built from $15 \times 15 \times 15$ unit cells of b-cristobalite.

Bibliography

[1] Bin Luan and Mark O Robbins. The breakdown of continuum models for mechanical contacts. *Nature*, 435(7044):929–932, 2005.