Lattice Dynamics

A project report submitted by

Shivansh Jaiswal

in partial fulfilment of the requirement for the award of the degree of

B.Tech

Indian Institute of Technology Jodhpur

Department of Metallurgical and Materials Engineering

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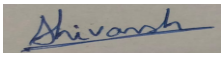
Declaration

I hereby declare that the work presented in this Project Report titled **Lattice Dynamics** submitted to the Indian Institute of Technology Jodhpur in partial fulfilment of the requirements for the award of the degree of B. Tech is a bonafide record of the work carried out under the supervision of **Dr Appala Naidu Gandi.** The contents of this Project Report in full or in parts, have not been submitted to, and will not be submitted by me to, any other Institute or University in India or abroad for the award of any degree or diploma.



Shivansh Jaiswal

B20MT041

Certificate

This is to certify that the Project Report titled **Lattice Dynamics** submitted by **Shivansh Jaiswal** to the Indian Institute of Technology Jodhpur for the award of the degree of **B. Tech**, is a bonafide record of the work done by him/her under my supervision. To the best of my knowledge, the contents of this report, in full or in parts, have not been submitted to any other Institute or University for the award of any degree or diploma.

Signature

Dr Appala Naidu Gandi

Abstract

Vesta software and understood making of a crystal lattice and representing volumetric data such as electron/nuclear densities, and crystal morphologies, monolayer representation, 2H variant, etc. The literature survey about the topic Lattice Dynamics, understood the PHON program which gives us output in form of phonon dispersion relation, and the concepts of Lattice Dynamics.

The basic command of Linux and working of the Linux OS and performed an exercise which will be useful for better understanding of the Linux.

Keywords: Lattice, Vesta, Phonon, Dispersion Relation, Linux, PHON program, Phonon dispersion relation.

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CHAPTER 1
INTRODUCTION AND BACKGROUND

1.1 Introduction to Vesta Software

Visualization for Electronic Structural Analysis (Vesta) is a 3D visualization program for structural models, volumetric data such as electron/nuclear densities, and crystal morphologies.

It helps us to improve our visualization of the structures.

1.2 Lattice Dynamics

Lattice Dynamics is the Study of the vibration of the atom in a crystal lattice. Crystal lattice dynamics is based on the concept of phonons, that is, weakly interacting waves of atomic (or ionic) vibrations and corresponding quasiparticles. A phonon is a definite discrete unit or quantum of vibrational mechanical energy, just as a photon is a quantum of electromagnetic or light energy.

A unit of vibrational energy that arises from oscillating atoms within a crystal

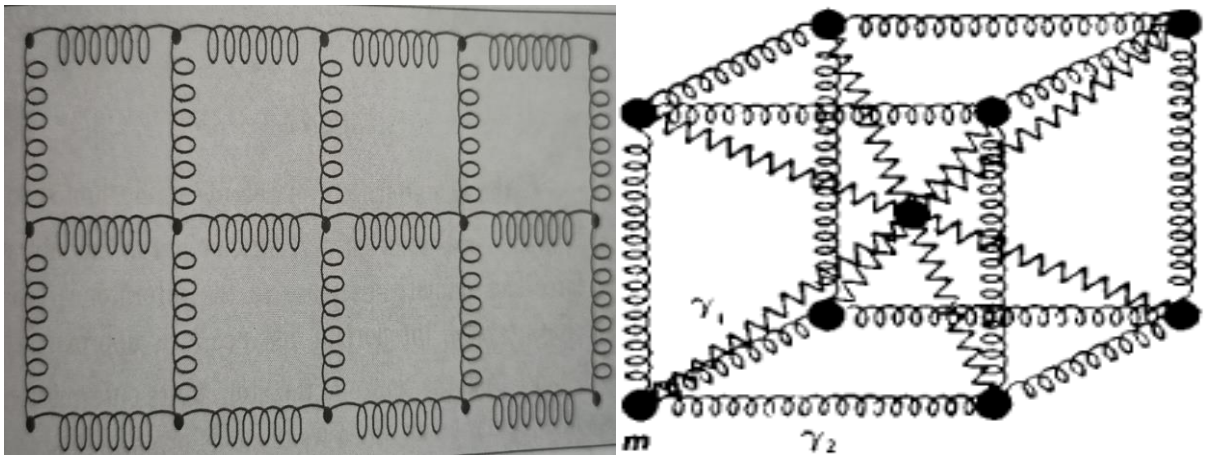

Fig. 1: Crystal Lattice

1.3 Introduction to Linux

Linux is an open-source operating system (OS). An operating system is the software that directly manages a system's hardware and resources, like CPU, memory, and storage.

CHAPTER 2
LITERATURE SURVEY

2.1 What is Lattice Dynamics

Lattice Dynamics is the Study of the vibration of the atom in a crystal lattice. Crystal lattice dynamics is based on the concept of phonons, that is, weakly interacting waves of atomic (or ionic) vibrations and corresponding quasiparticles.

2.2 Historical Aspect of Lattice Dynamics

The story of lattice dynamics begins in 1905, with Einstein's confirmation, via his theory of Brownian motion, that atomic vibration really do exist.

After that many scientists had used the concept of lattice dynamics to get a better understanding at the concepts and proposed many theories for better understanding of Lattice Dynamics.

2.3 Lattice Vibration

Every atom has a tendency to vibrate about their mean position at temperature above zero Kelvin. The mean position is referred as the Bravais lattice site. These vibrations occur due to interatomic interactions. As the atoms in the solids are present at lattice sites, so these vibrations are called lattice vibrations.

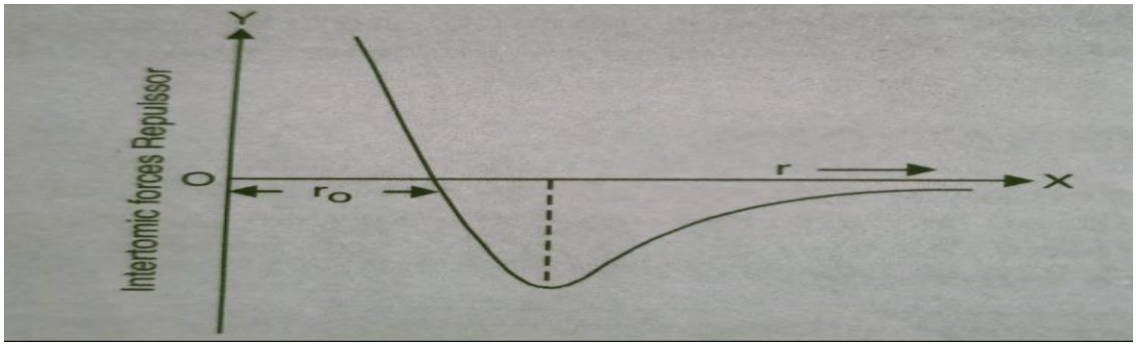

Fig. 2: Graph between Interatomic force vs interatomic distance

2.4 Why we have to study Lattice Dynamics

Traditional crystallography often leads to the image of atoms being held in static positions through stiff chemical bonds. Yet crystallographic measurements tell us that atoms can be vibrating with an amplitude that can be of order of 10% of an interatomic distance.

2.5 Applications of Lattice Dynamics

The propagation of sound waves in crystals are a practical example of the application of lattice dynamics, as also is the interaction of materials with light. For example, the absorption of certain frequencies in the infrared spectral region is directly due to the existence of specific lattice dynamics motions.

Lattice dynamics also gives us properties such as thermodynamics, superconductivity, phase transitions, thermal conductivity, and thermal expansion.

2.6 Phonons

A phonon is the quantum mechanical description of an elementary vibrational motion in which a lattice of atoms or molecules uniformly oscillates at a single frequency. In classical mechanics this designates a normal mode of vibration.

A packet of these waves can travel throughout the crystal with a definite energy and momentum, so in quantum mechanical terms the waves can be treated as a particle, called a phonon.

2.7 Phonon Dispersion Relations

The phonon dispersion relations are defined as the *k* dependence of the frequencies, ω(k,j) of the normal modes for all branches *j* and selected directions in the crystal.

For a one-dimensional alternating array of two types of ion or atom of mass m_1, m_2 repeated periodically at a distance *a*, connected by springs of spring constant *K*, two modes of vibration.

$$\omega_{\pm}^2 = K\left(\frac{1}{m_1}+\frac{1}{m_2}\right) \pm K\sqrt{\left(\frac{1}{m_1}+\frac{1}{m_2}\right)^2 - \frac{4\sin^2\frac{ka}{2}}{m_1 m_2}},$$

Fig.3: Expression for frequency

The connection between frequency and wavevector, $\omega = \omega(k)$, is known as a dispersion relation. The plus sign results in the so-called *optical* mode, and the minus sign to the *acoustic* mode.

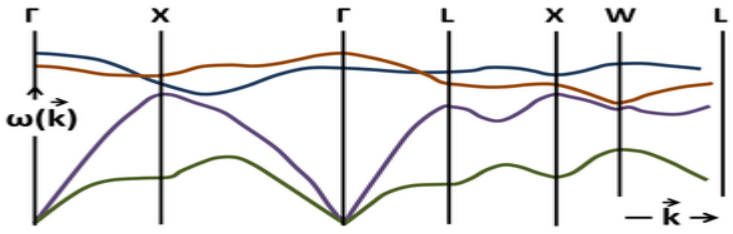

Fig.4: Phonon Dispersion relation

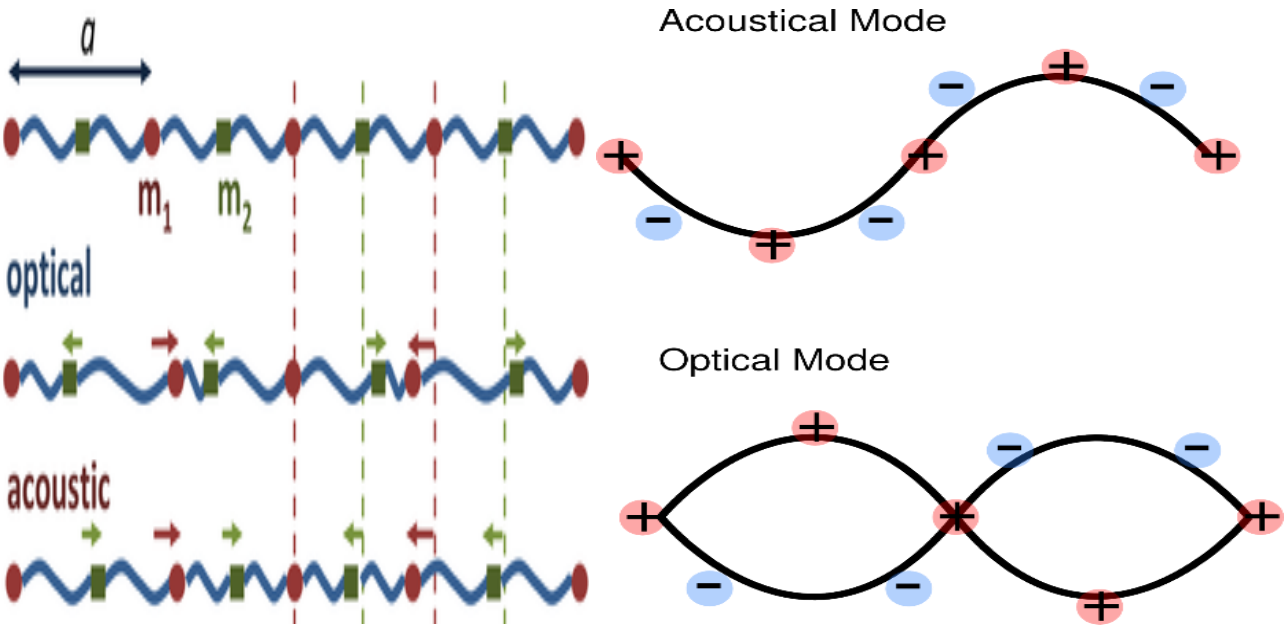

Fig.5: Aucostic and Optical Waves

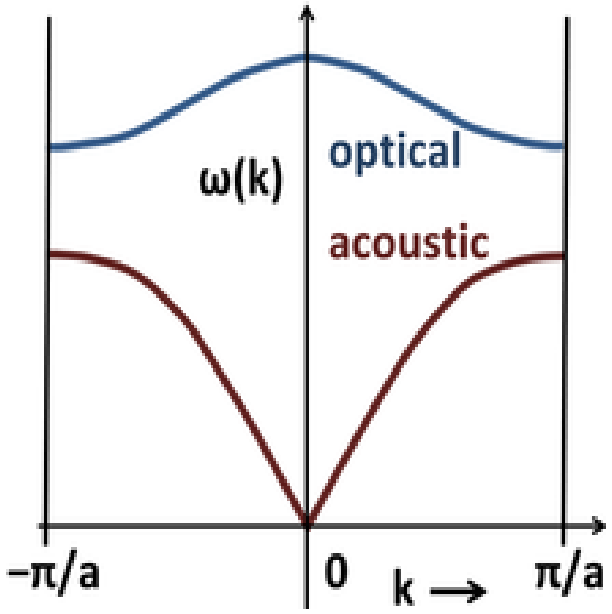

Fig.6: Phonon Dispersion Relation using Optical and Aucostic Waves

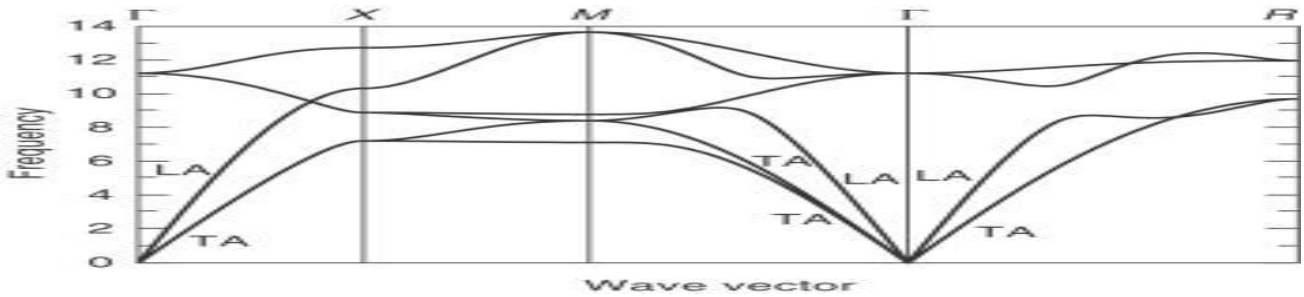

Fig.7: Phonon Dispersion relation for Aluminuim

2.8 Force Constants and 2-nd order force constants

A force constant defined as a second energy derivative relative to internal coordinates near the equilibrium position, Fij = d2E/dqi*dqj, is obtained most simply by the double differentiation in various points of the two-dimensional grid of qi and qj values.

Potential energy of phonon system is represented as functions of atomic positions:

The second order force constants is given by: $\Phi_{\alpha\beta}$

$$\Phi_{\alpha\beta}(jl, j'l') = \frac{\partial^2 V}{\partial r_\alpha(jl)\partial r_\beta(j'l')} = -\frac{\partial F_\beta(j'l')}{\partial r_\alpha(jl)},$$

Fig.8: Expression for 2nd order force constant

2.9 PHON Program

- The program PHON calculates force constant matrices and phonon frequencies in crystals. From the frequencies it also calculates various thermodynamic quantities, like the Helmholtz free energy, the entropy, the specific heat and the internal energy of the harmonic crystal.
- The procedure is based on the small displacement method, and can be used in combination with any program capable to calculate forces on the atoms of the crystal. In order to examine the usability of the method, here two examples: metallic Al and insulating MgO.

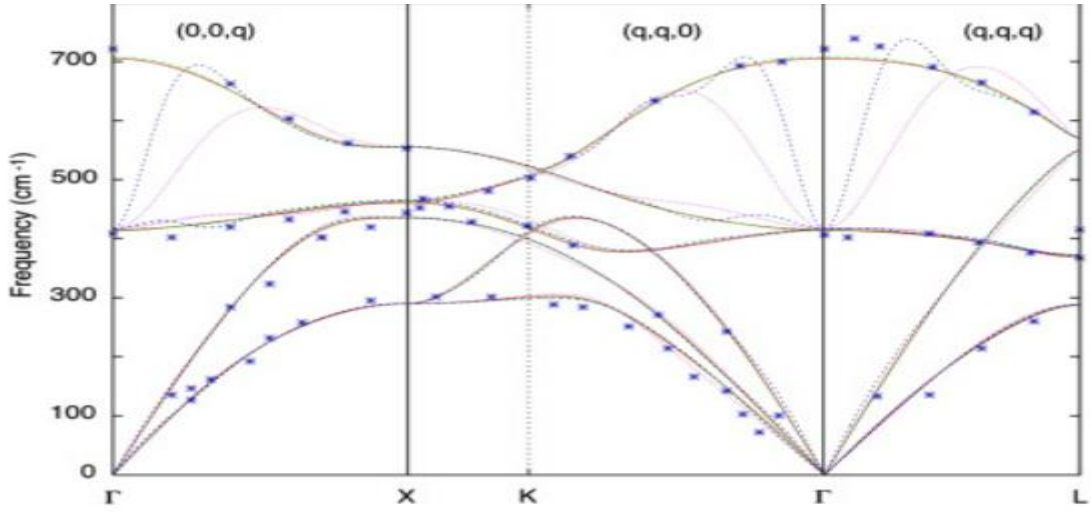

Fig.9: Phonon Dispersion Relation of MgO using the PHON program

CHAPTER 3

PROBLEM DEFINATION AND OBJECTIVE

3.1 Learning Vesta Software

Learn Vesta Software and make structures on it and getting familier woth the interface, making poscar, incar files and see the visual representation of charge density, 2h varient, forming a mono-layer.

3.2 Literature Survey

Getting familiar with the topic, reading research papers and presenting my finding on the basis of them.

3.3 Introduction to Linux OS

Learning basics of the linux and performing an exercise for getting familiar to the OS.

CHAPTER 4

METHEODOLOGY

4.1 Vesta Software

Reading the vesta module and watching vesta tutorial for construction of structures and showing properties such as charge density.

4.2 Literature Survey

Reading different paper's based on lattice dynamic and phon, phonon dispersion relation, PHON Program, and understand them.

4.3 Introduction to Linux

Reading the manual for linux, and practise basic operations on a linux device.

CHAPTER 5

THEORETICAL/NUMERICAL/EXPERIMENTAL FINDINGS

5.1 Using Vesta

Making a unit cell : GaAs

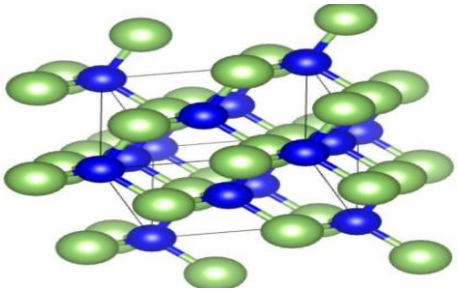

Fig.10: Unit Cell of GaAs

Making a unit cell, atomic planes and direction

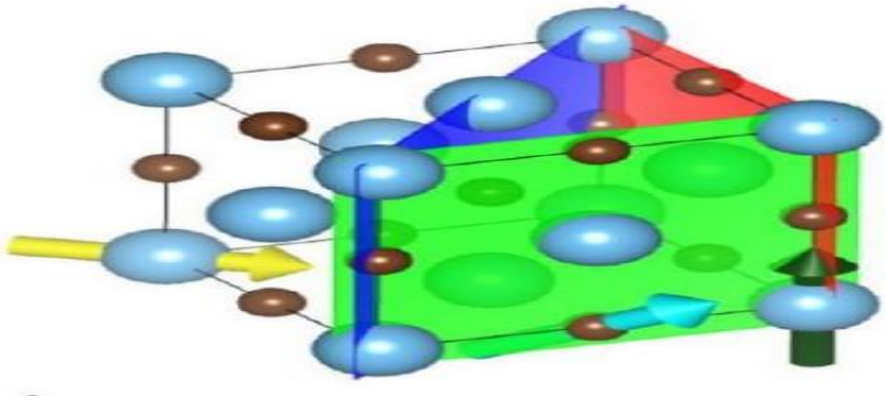

Fig.11: Unit cell, atomic planes and direction

Charge Density of NaCl structure using vesta

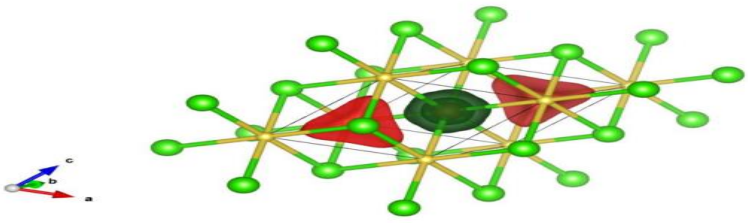

Fig.12: Charge Density of NaCl structure

Charge density of Si atom using vesta

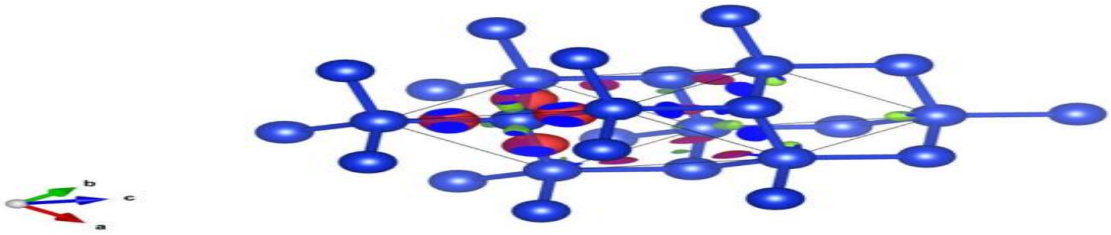

Fig.13: Charge Density of Si

Making 2H variant Crystal of WSe_2

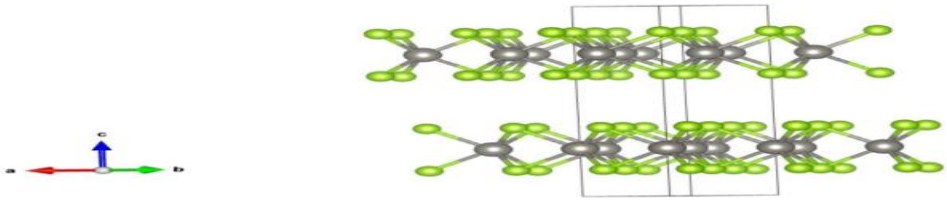

Fig.14: 2H variant Crystal of WSe_2

Monolayer formation of WSe2

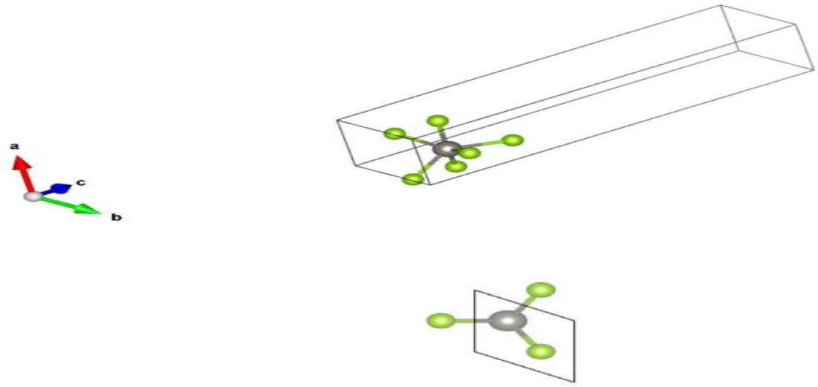

Fig.15: Monolayer of WSe2

Combining two monolayers MoSe2_WSe2

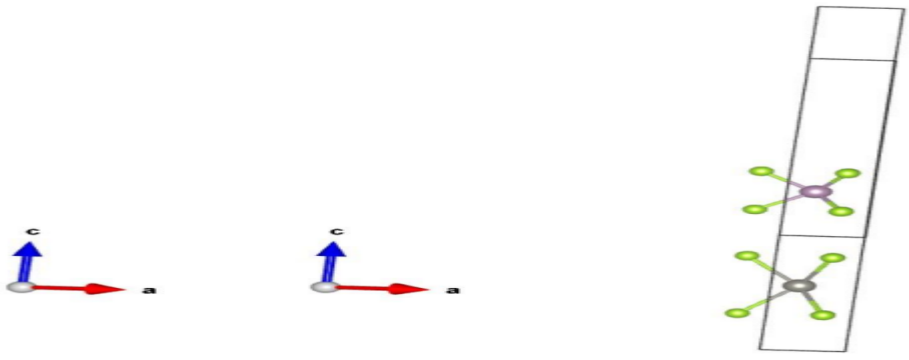

Fig.16: Combined Monolayer of MoSe2_WSe2

5.2 In Literature

$$U_{\text{harm}} = E_{\text{perf}} + \frac{1}{2}\sum_{ls\alpha,l't\beta}\Phi_{ls\alpha,l't\beta}u_{ls\alpha}u_{l't\beta}$$

Fig.17: Expression for harmonic Potential

- In order to calculate the energy we assume that the potentials are treated as the harmonic potentials, this assumptions is valid as long as the atoms remain close to equilibrium position.
- The expression for potential is obtained by using the Taylor's expansion and we found that the potential is proportional to displacement square and gives the quadratic term.
- Higher order terms are neglected as we as assuming the displacement about there mean position to be less.

Understanding the expression in depth

- Consider a solid consisting of N atoms, each of mass mi, with position ri. The equilibrium position is ri0 .Each atom can vibrate about its equilibrium position. The displacement from the equilibrium position $\xi_{i\alpha} \equiv x_{i\alpha} - x_{i\alpha}^{(o)} \qquad \text{where } \alpha = 1, 2, \text{ or } 3$
- Since the displacements are small, we can expand the potential energy taylor's series:

$$V = V_o + \sum_{i\alpha}\left[\frac{\partial V}{\partial x_{i\alpha}}\right]_o \xi_{i\alpha} + \frac{1}{2}\sum_{i\alpha,j\gamma}\left[\frac{\partial^2 V}{\partial x_{i\alpha}\partial x_{j\gamma}}\right]_o \xi_{i\alpha}\xi_{j\gamma} + \cdots$$

- In the expression I and j go from 1 to n; and alpha and gamma go from 1 to 3.
- The derivatives are evaluated at the equilibrium positions of atoms.
- The first term Vo is the potential energy when the atoms are in their equilibrium configuration.

$$[\partial V/\partial x_{i\alpha}]_o = 0$$

- Since Vo is the minimum value of V the first derivative must be equals to zero.
- That is there is no force on any atom in the equilibrium configuration. So the first term in the Taylor series vanishes and we get the expression

$$V = V_o + \frac{1}{2}\sum_{i\alpha,j\gamma} A_{i\alpha,j\gamma}\xi_{i\alpha}\xi_{j\gamma}$$

It can also be given as:

$$U_{\text{harm}} = E_{\text{perf}} + \frac{1}{2}\sum_{ls\alpha,l't\beta}\Phi_{ls\alpha,l't\beta}u_{ls\alpha}u_{l't\beta}$$

5.3 In Linux, Exercise to find the optimal lattice parameter using Linux

The exercise was to find the optimal lattice parameter for which we can get the optimal energy. For this, we used the formula:

$$B = \frac{1}{9V_0}\frac{\partial^2 E^{tot}}{\partial \gamma^2}$$

We used the Linux operation and a Linux software which will find and gnuplot for plotting the curve between Lattice parameter and energy.

```
9.2 !    total energy              =     -15.73969636 Ry
9.3 !    total energy              =     -15.76225273 Ry
9.4 !    total energy              =     -15.78155701 Ry
9.5 !    total energy              =     -15.79780536 Ry
9.6 !    total energy              =     -15.81120623 Ry
9.7 !    total energy              =     -15.82211624 Ry
9.8 !    total energy              =     -15.83064586 Ry
9.9 !    total energy              =     -15.83693026 Ry
10.0 !    total energy              =     -15.84130269 Ry
10.1 !    total energy              =     -15.84383739 Ry
10.2 !    total energy              =     -15.84473346 Ry
10.3 !    total energy              =     -15.84411890 Ry
10.4 !    total energy              =     -15.84220359 Ry
10.5 !    total energy              =     -15.83905059 Ry
10.6 !    total energy              =     -15.83481246 Ry
10.7 !    total energy              =     -15.82959860 Ry
10.8 !    total energy              =     -15.82351561 Ry
10.9 !    total energy              =     -15.81665362 Ry
11.0 !    total energy              =     -15.80908508 Ry
11.1 !    total energy              =     -15.80090696 Ry
11.2 !    total energy              =     -15.79222481 Ry
```

Fig.18: Energy respective to the lattice parameter

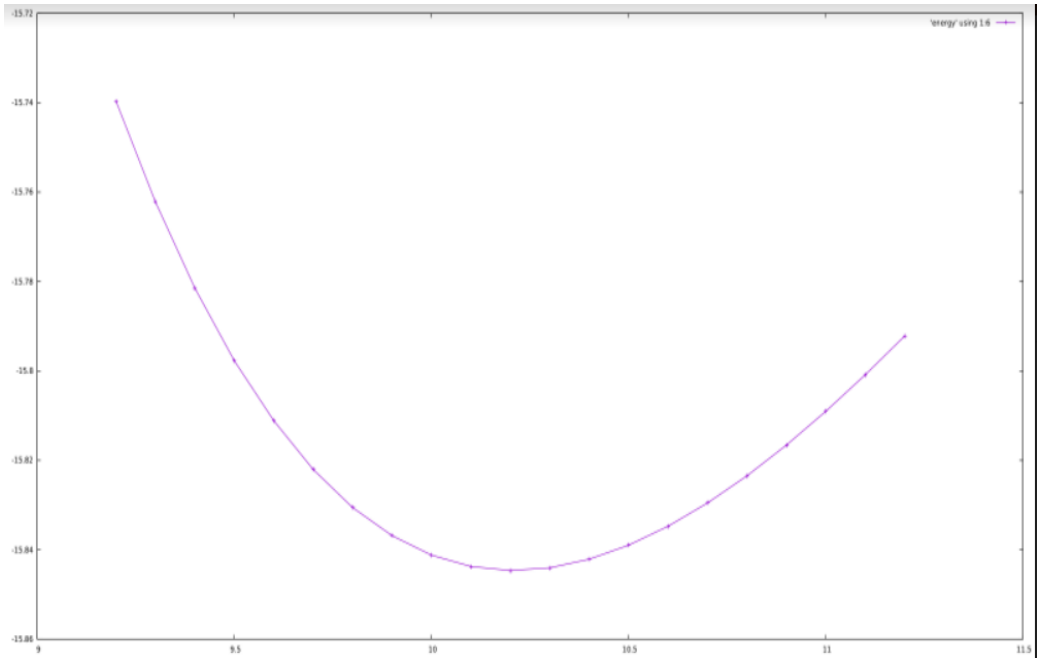

Fig.19: Graph between Lattice parameter and Energy

By the graph we can conclude that the optimal lattice parameter is 10.2(approx.)

CHAPTER 6

SUMMARY

Using Vesta software forming different unit cell and shown many volumetric data such as electron/nuclear densities, and crystal morphologies, monolayer representation, 2H variant, etc.

Literature survey for lattice dynamics Understanding the concepts in depth and understanding the PHON program which helps us to find the phonon dispersion relation.

Using Linux finding the optimal Lattice parameter and understood the basic functioning of the Linux OS.

CHAPTER 7

REFERENCES

- Article on Science direct webpage about lattice Dynamics
  Link: https://www.sciencedirect.com/topics/chemistry/lattice-dynamics#:~:text=Introduction,be%20described%20as%20a%20particle).
- Introduction to Lattice Dynamics Book by Martin T. Dove
- Lattice Dynamics Book by A.A. Maradudin
- Article on Neuro Science website
  Link: https://www.neutron-sciences.org/articles/sfn/pdf/2011/01/sfn201112007.pdf
- Wikipedia
- Artice on Phonon Dispersion relation
  Link : https://www.sciencedirect.com/topics/engineering/phonon-dispersion
- Vesta learning module
  Link : https://vestaevv.com/wp-content/uploads/2021/12/Vesta-Learning-Management-System.pdf
- Linux learning module Basics of linux
  Link: https://www.hostinger.in/tutorials/linux-commands
- Introduction to solid state Book by Charles Kittles