Mechanical Behaviour study using first principle calculations

A project report submitted by

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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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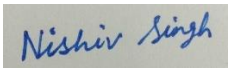
Declaration

I hereby declare that the work presented in this Project Report titled **Mechanical behaviour study using first principles calculations** 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.



Nishiv Singh

B20MT029

Certificate

This is to certify that the Project Report titled **Mechanical behaviour study using first principles calculations**, submitted by **Nishiv Singh** 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

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Abstract

This report includes the work done on the topic **Mechanical Behaviour study using first principle calculations,** a literature survey is done on the topic, and the paper includes methods used for calculations, the foremost work was preparing input files for further calculations, for which ***Vesta*** software is used, using basic data of a compound. Certain topics are explained with necessary derivation if required with calculations, The input files are used to calculate various mechanical properties like elastic constants and bulk modulus etc. which was carried on ***Linux*** operating system.

Keywords:

- First principle calculations
- Quantum mechanics
- Bulk modulus
- Vesta software
- Linux operating system
- Lattice parameters
- Unit cell
- Stiffness tensor
- Stress-strain curve
- Voigt notation
- Elastic energy
- Homogenous Deformation Method
- Optimal lattice parameter
- Hooke's law

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CHAPTER 1

INTRODUCTION AND BACKGROUND

Approaching the field of Mechanical behaviour study from a theoretical or computational angle can be a very challenging task to undertake. For the most part, the way this is done is to pick a particular macroscopic phenomenon, which has been well studied experimentally, and to build empirical, or semi-empirical, models to describe the experimentally observed results. This often provides a good understanding of the physics of the system under study, and it is often possible to interpolate or extrapolate these models in order to predict the behaviour of systems under conditions not yet tested experimentally. However, the predictive power of such an approach can be severely limited.

The *first principles* approach to Mechanical behaviour study is entirely different from this. It starts from what we know about all condensed matter systems - that they are made of atoms, which in turn are made of a positively charged nucleus, and a number of negatively charged electrons. The interactions between atoms, such as chemical and molecular bonding, are determined by the interactions of their constituent electrons and nuclei. All of the physics of materials arises ultimately from these basic interactions. If we can model these interactions accurately, then all of the complex physical phenomena that arise from them should emerge naturally in our calculations.

The physics that describes the interaction of electrons and nuclei that is relevant to most problems in this area is actually relatively simple. There are only two different types of particle involved, and the behaviour of these particles is mostly governed by basic quantum mechanics. What makes first principles calculations difficult is not so much the complexity of the physics, but rather the size of the problem in terms of a numerical formulation. The development of accurate and efficient theoretical and computational techniques for dealing with so many particles is therefore central to the ongoing research in this field

CHAPTER 2

LITERATURE SURVEY

2.1 First Principles calculations

"First principles calculation" is a method to calculate physical properties directly from basic physical quantities such as the mass and charge, Coulomb force of an electron, etc. based on the principle of quantum mechanics.
Mechanical properties e.g. ideal strength and elastic constants are accessible directly by first-principles calculations, such methods may predict the complex mechanical properties by extracting appropriate calculable parameters (e.g., the ratio of bulk modulus to shear modulus, the formation energies of and interaction energies between lattice defects)

2.2 Stacking Faults

In crystallography, a **stacking fault** is a planar defect that can occur in crystalline materials. Crystalline materials form repeating patterns of layers of atoms. Errors can occur in the sequence of these layers and are known as stacking faults. Stacking faults can arise during crystal growth or from plastic deformation.

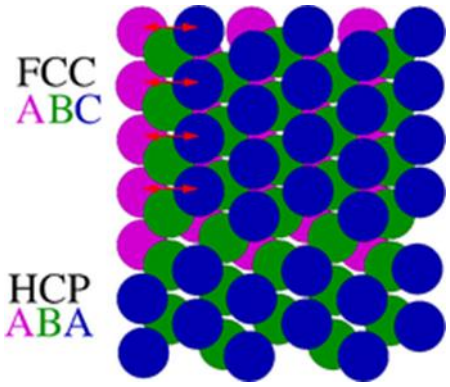

Figure 2.1: Comparison of fcc and hcp lattices, explaining the formation of stacking faults in close-packed crystals

2.3 Surface Energy

surface energy quantifies the disruption of intermolecular bonds that occurs when a surface is created.
The surface energy may therefore be defined as the excess energy at the surface of a material compared to the bulk, or it is the work required to build an area of a particular surface.

2.4 Crystallographic defects

Crystallographic defects are interruptions of regular patterns in crystalline solids. They are common because positions of atoms or molecules at repeating fixed distances determined by the unit cell parameters in crystals, which exhibit a periodic crystal structure, are usually imperfect.

2.5 Stiffness Tensor

Stress and strain are related to each other by Hooke's Law where the strain is assumed to be sufficient small that stress and strain depend linearly on each other. Such a medium is called linear elastic. In its general form Hooke's law reads:

$$[\boldsymbol{\sigma}] = [\mathsf{C}][\boldsymbol{\varepsilon}] \qquad \text{or} \qquad \sigma_i = C_{ij}\varepsilon_j \,.$$

It is often useful to express the anisotropic form of Hooke's law in matrix notation

$$[\boldsymbol{\sigma}] = \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix} \equiv \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix}; \qquad [\boldsymbol{\varepsilon}] = \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{23} \\ 2\varepsilon_{13} \\ 2\varepsilon_{12} \end{bmatrix} \equiv \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix}$$

Then the stiffness tensor (c) can be expressed as

$$[\mathsf{c}] = \begin{bmatrix} c_{1111} & c_{1122} & c_{1133} & c_{1123} & c_{1131} & c_{1112} \\ c_{2211} & c_{2222} & c_{2233} & c_{2223} & c_{2231} & c_{2212} \\ c_{3311} & c_{3322} & c_{3333} & c_{3323} & c_{3331} & c_{3312} \\ c_{2311} & c_{2322} & c_{2333} & c_{2323} & c_{2331} & c_{2312} \\ c_{3111} & c_{3122} & c_{3133} & c_{3123} & c_{3131} & c_{3112} \\ c_{1211} & c_{1222} & c_{1233} & c_{1223} & c_{1231} & c_{1212} \end{bmatrix} \equiv \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{bmatrix}$$

Figure 2.2 Stiffness tensor in matrix form

2.6 Stress-Strain Curve

When we study solids and their mechanical properties, information regarding their elastic properties is most important. We can learn about the elastic properties of materials by studying the stress-strain relationships, under different loads, in these materials.

The material's stress-strain curve gives its stress-strain relationship. In a stress-strain curve, the stress and its corresponding strain values are plotted.

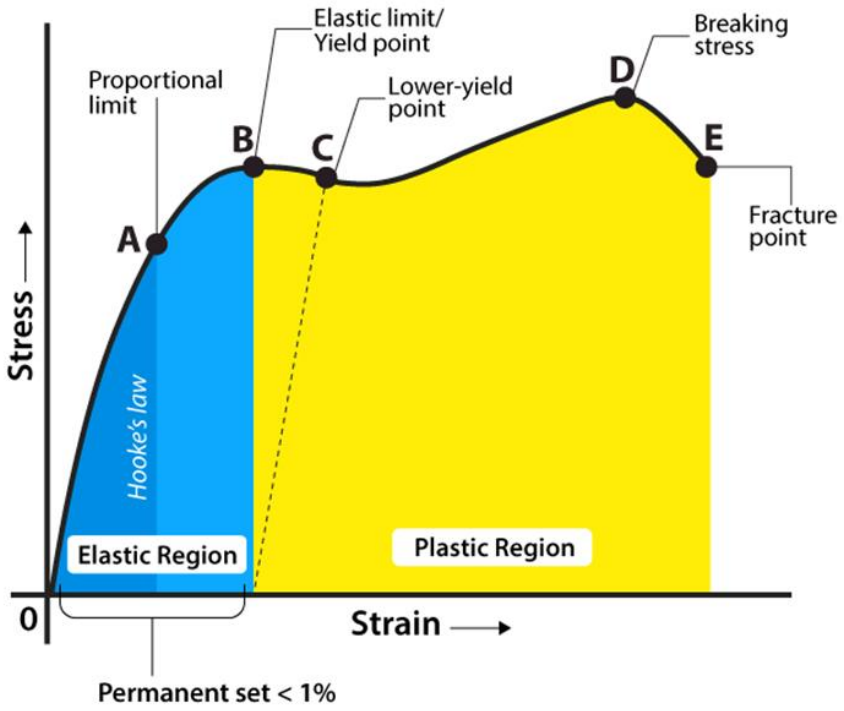

Figure 2.3 Stress-Strain Curve

2.7 Elastic Energy

Elastic energy is the mechanical potential energy stored in the configuration of a material or physical system as it is subjected to elastic deformation by work performed upon it. Elastic energy occurs when objects are impermanently compressed, stretched or generally deformed in any manner.

The elastic energy density is given by $$E^{\mathrm{ela}} = \frac{1}{2}\sum_{ijkl} \mathrm{C}_{ijkl}\epsilon_{ij}\epsilon_{kl}.$$

2.8 Homogenous Deformation Method (HDM)

This method is used to determine elastic constants of a crystal structure.

For a given strain tensor it is possible to write total energy in terms of elastic tensor elements and γ.[1]

$$E^{\mathrm{tot}} = E^0 + \frac{1}{2}\gamma^2 \sum_{ijkl} \mathrm{C}_{ijkl}\epsilon_{ij}\epsilon_{kl}$$

For calculating the complete elastic stiffness tensor of a crystal the same procedure is repeated using different homogeneous strain tensors

CHAPTER 3

PROBLEM DEFINITION AND OBJECTIVES

3.1 Problem

To calculate various mechanical properties i.e., elastic constants, bulk modulus from basic microscopic quantities i.e., mass, charge, lattice parameter

3.2 Objectives

1. Getting familiar with the relevant literature.
2. Preparation of input files for the calculations.

CHAPTER 4

METHODOLOGY

4.1 Preparation of input files

Vesta software is used to prepare input files which are to be used for calculations, the software uses basic data about the property to be determined, e.g., for creating unit cell lattice parameters should be given along with position of atoms and crystal structure, unit cell image generated by *Vesta* is shown below:

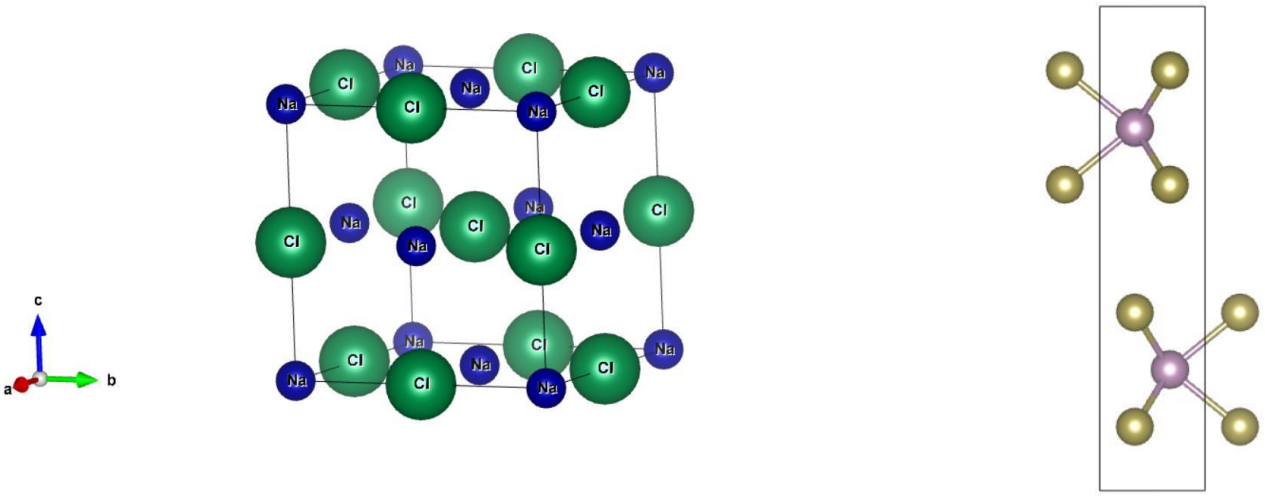

Figure 4.1 Unit cells of NaCl, MoTe2

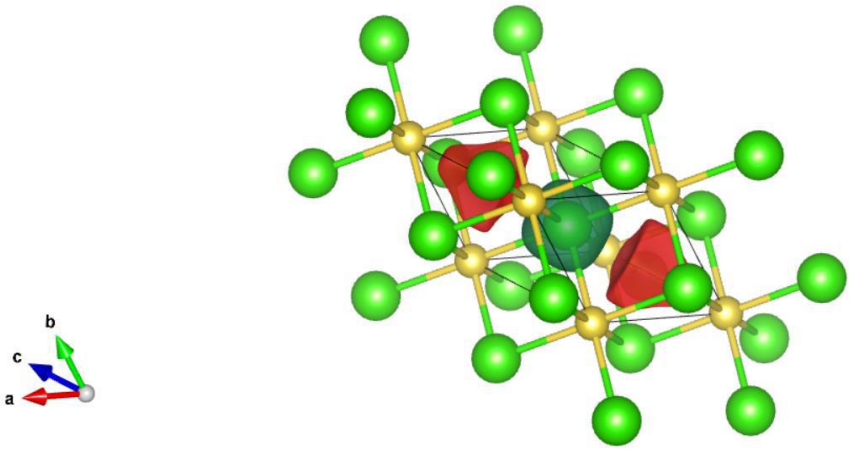

Figure 4.2 charge density unit cell of NaCl

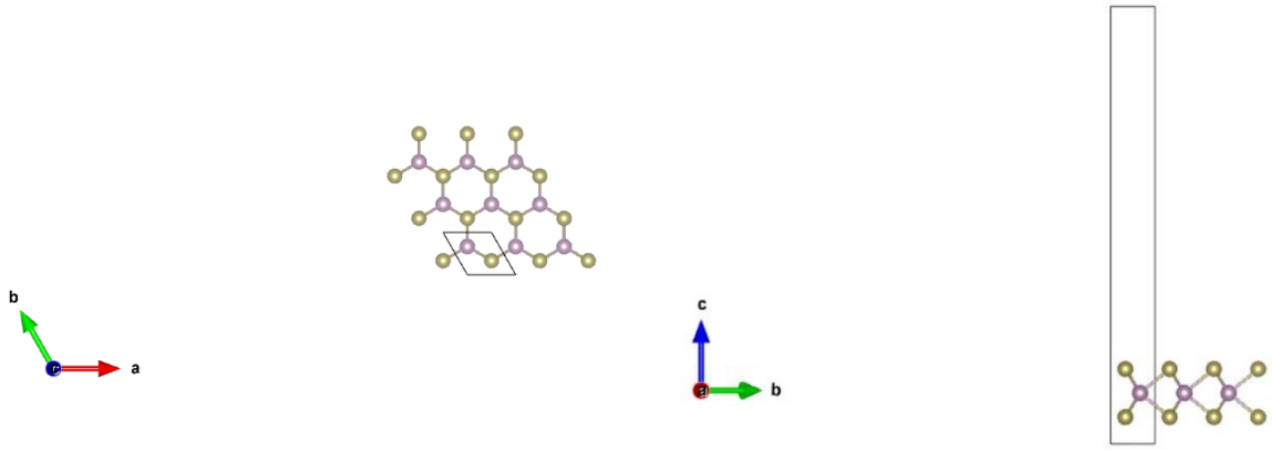

Figure 4.3 Monolayer unit cell of MoTe2

4.2 Calculation using *Linux* operating system

The input are then used to calculate various mechanical properties by using *linux* operating system , the operating system is well known for its security , various commands are used to do necessary calculation like the work done on linux includes calculation of energy of a unit cell from given lattice parameter , calculating optimal lattice parameter using Energy vs Lattice parameter graph etc.

CHAPTER 5

THEORETICAL/NUMERICAL/EXPERIMENTAL FINDINGS

5.1 Elastic energy for cubic crystal

For a cubic crystal structure

C11 = C22 = C33

C12 = C21 = C31 = C13 = C23 = C32

C44 = C55 = C66

rest are 0.

i.e.,

$$C = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix},$$

Thus, in expanded form the total energy of a cubic crystal is given by:

$$E^{\text{tot}} = E^{\circ} + \frac{1}{2}\mathrm{C}_{11}(\epsilon_1^2 + \epsilon_2^2 + \epsilon_3^2) + \mathrm{C}_{12}(\epsilon_1\epsilon_2 + \epsilon_2\epsilon_3 + \epsilon_3\epsilon_1) + \frac{1}{2}\mathrm{C}_{44}(\epsilon_4^2 + \epsilon_5^2 + \epsilon_6^2)$$

5.2 Calculating optimal lattice parameter of given unit cell in input file

Different energies are calculated at corresponding lattice parameter and a graph is plotted between lattice parameter and energies, here lattice constants are in the unit of Angstrom and energy in the unit of Ry (2.1798741E-18 J)

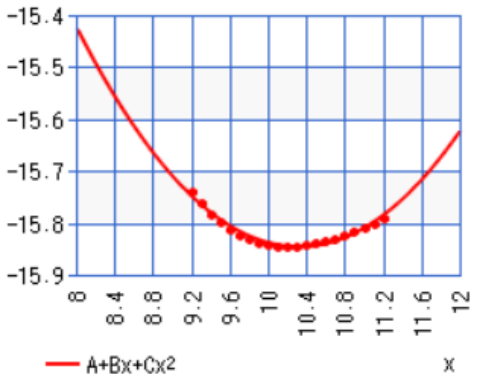

Figure 5.1 Energy vs Lattice parameter graph

Energy is extrapolated as a second order polynomial of lattice parameter, from the graph the energy obtained is

E_a = -7.4979 + (-1.619)a + (0.078497)a^2

For minimum energy , dy/dx = 0

d(A+Bx+Cx^2)/dx = 0

2Cx+B = 0

x = -B/2C

The equilibrium lattice constant is ao = -(-1.619)/2*(0.078497)

= 10.313 A

CHAPTER 6

SUMMARY

Mechanical properties which are the macroscopic properties can be easily be theoretically determined by using first principle calculations, in which basic properties of the basic unit i.e., mass, charge, lattice parameters etc.

The calculation for these properties requires some specific data about the unit cell, for this purpose a software named *Vesta* is used to get the input files for further calculations, various input files are made e.g., separating a monolayer of a molecule from the unit cell of MoTe2 and then using this monolayer with a monolayer of MoS2 to create a complete new heterolayer unit cell.

Certain terms are also discussed which are necessary for further calculations e.g., Surface Energy, Stiffness Tensor, Elastic Energy, Homogenous Deformation Method.

Homogenous Deformation Method is used to determine elastic constants from the elastic energy equation, and from elastic constants further mechanical properties like bulk modulus, stress- strain ratio can be determined.

Then a *Linux* based operating system is used for final calculations which are calculating optimal lattice, energy of Ni unit cell.

- ## References

[1] Dr.Appala Naidu Gandi , Martensitic Transformation in TiNi Based Shape Memory Alloys: A First Principles Study, pp. 71–73 ,2013
https://scholar.google.com/citations?view_op=view_citation&hl=en&user=1wv6BE8AAAAJ&cstart=20&pagesize=80&citation_for_view=1wv6BE8AAAAJ:u5HHmVD_uO8C