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MECHANICAL STABILITY OF BODY-CENTERED CUBIC IRON IN BORN-VON KÁRMÁN PARAMETER SPACE USING EVOLUTIONARY ALGORITHMS

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AMIR HUSEN

2024

To my family,

who have always been patient and supportive of me.

Thank you.

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AMIR HUSEN

THESIS

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Abstract

This study aims to assess the mechanical stability of body-centered cubic (BCC) structure, focusing on pure iron as a representative case. The primary approach involves utilizing phonon dispersion curves analysis to gain insights into the vibrational properties and overall stability of the crystal lattice through a multi-faceted computational approach. The goal of the study is to find the regions (pockets) in Born-von Kármán (BvK) parameter space where the crystal is stable for certain temperature and pressure.

This involves setting up the crystal parameters, creating a body-centered cubic (BCC) crystal with specific lattice parameters (2.86 for iron) establishing force constants, and employing Phonopy for phonon dispersion analysis. We developed a genetic algorithm to investigate the mechanical stability of body-centered cubic (BCC) iron in reduced BvK parameter space. For each genetic solution, we calculate the phonon dispersion relations by computing the dynamical matrix at various grid points across the Brillouin Zone. We then evaluate the stability of each solution by measuring deviations from predefined mechanical stability conditions.

Introduction of the RMSE metric provides a quantitative assessment of the accuracy of the computational model. The imaginary frequencies identified during the phonon dispersion analysis highlight potential areas of instability in the BvK space, and application of a genetic algorithm serves as an innovative approach to optimize the model and enhance its accuracy.

The comprehensive nature of this analysis positions it as a foundational study for further exploration into the mechanical stability of metallic crystals, with potential applications in materials science and engineering.

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Chapter 1

Introduction

1.1 Introduction

Iron, an elemental metal with pivotal roles in both natural and engineered systems, presents intriguing properties crucial to various fields, including metallurgy, geophysics, and materials science [14, 31, 45]. Specifically, body-centered cubic (BCC) iron exhibits complex behavior under different environmental conditions such as temperature and pressure, pivotal in understanding its structural transitions and mechanical stability [21, **?**]. This research aims to delve deeper into the mechanical stability of BCC iron using advanced computational techniques, focusing on phonon dispersion analysis to explore its vibrational properties and lattice dynamics. This inquiry incorporates setting specific lattice parameters for iron, exploring interactions among nearest neighbors, and applying phonon dispersion analyses using Phonopy software. The integration of evolutionary algorithms, particularly genetic algorithms, serves to optimize the accuracy by refining the Born-von Kármán (BvK) parameters, offering potential enhancements in predicting the conditions under which BCC iron remains mechanically stable.

1.2 Rationale

The study presented in this thesis is significant for several reasons, primarily focusing on the mechanical stability of body-centered cubic (BCC) iron within the Born-von Kármán (BvK) parameter space using evolutionary algorithms. Here are the key points highlighting its importance:

Advanced Understanding of BCC Iron

Iron is a fundamental material in numerous industrial applications due to its mechanical and magnetic properties [27]. The study's focus on the mechanical stability of BCC iron helps clarify how iron behaves at the atomic level, particularly in its BCC phase, which is crucial for its applications in engineering and technology.

Phonon Behavior Insights

Phonons are critical in understanding the thermal and mechanical properties of materials, impacting various aspects such as thermal conductivity, mechanical strength, and thermal expansion [60]. By studying phonon dispersion in BCC iron, this research contributes to the broader field of materials science, providing insights into the vibrational properties of iron's crystal lattice.

Advancement in Computational Materials Science

The use of evolutionary algorithms, such as genetic algorithms, to optimize computational models represents a significant advancement in the field of computational materials science [36]. These methods allow for more accurate and efficient simulations, reducing the time and cost compared with experimental methods. By improving the accuracy of predictive models that determine the stability of crystal structures, this research facilitates the design of new materials and the enhancement of existing ones. Better predictive models aid in understanding how materials will behave under stress or in extreme conditions, which is vital for applications ranging from aerospace to civil engineering.

Foundation for Further Research

The comprehensive analysis conducted in this study serves as a foundational research that could be built upon for further exploration into the stability of metallic crystals. This can potentially lead to new discoveries in material properties and the development of new

materials with tailored characteristics.

Overall, the research contributes significantly to the field of computational materials science by enhancing the understanding of the fundamental properties of iron, a critical industrial material, using sophisticated computational models.

1.3 Background

1.3.1 Crystal

Crystals are solid substances that have a uniform structure, with atoms or group of atoms, arranged in a regular and organized pattern throughout a three-dimensional space (Fig. 1.1). The atomic arrangement inside a small volume of a crystal is identical to that in any other similar region of the crystal, with the exception of localized errors or flaws that may occur during the crystal's formation or be intentionally introduced. The crystal structure of solids has a significant role in determining their chemical and physical properties [48]. The examples of crystals are table salt (NaCl), diamond etc.

Two terms are used to describe the crystal structure- (1) lattice and (2) basis (or motif).

Bravais Lattice: The Bravais lattice is a fundamental idea used to describe every crystalline solid. A Bravais lattice is a periodic arrangement of discrete points that exhibits identical appearance and orientation when viewed from any place within the lattice (Fig. 1.2) [4]. The points in a Bravais lattice are called lattice points and all lattice points can be

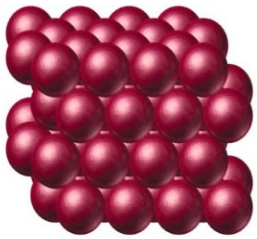


Figure 1.1: Crystalline solid

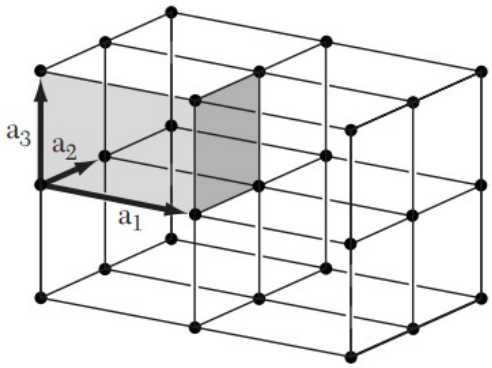


Figure 1.2: A portion of 3-D Barvais lattice

described with the position vectors $\mathbf{R}$ that can be expressed as

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 \ , \tag{1.1}$$

where n_1, n_2, and n_3 are integers and $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ are three vectors that are not all coplanar. The vectors $\mathbf{a}_i$ (i = 1, 2, 3) are referred to as primitive vectors and are responsible for generating or spanning the lattice. The volume of the parallelepiped $\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3$ is the smallest volume that can be used as a building block for the crystal structure. The primitive translation vectors are often used to define the crystal axes, which comprise three adjacent edges of the primitive parallelepiped [20].

Basis/Motif: A basis is an atom, or a set of atoms arranged in such a way that each basis within a given crystal is identical to every other basis in terms of composition, arrangement, and orientation. A crystal structure is composed of a basis situated at every point of a Bravais lattice. In general, crystal structure can be described as,
Crystal structure = lattice + basis (Fig 1.3).

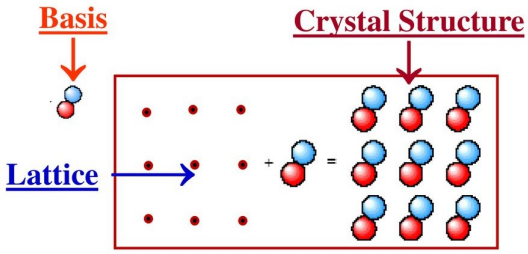


Figure 1.3: Crystal structure

1.3.2 Phonon

The idea of phonon was first introduced by soviet physicist Igor Tamm in 1932. The term 'phonon' was originated from the Greek word 'phone', which means sound or voice, as long-wavelength phonons are accountable for sound generation.

Phonons are conceptualized as quasi-particles [40] that encapsulate the collective vibrational modes of atoms within a crystal lattice. These entities play a pivotal role in delineating various thermal properties of solids, such as heat capacity and thermal conductivity [37, 16, 8], as well as electrical properties including electrical conductivity [30] and superconductivity [20]. Analogous to the wave functions of a harmonic oscillator in quantum mechanics, phonons represent the quantized states of these vibrational modes, but they span multiple dimensions to reflect the coordinated motion of myriad atoms across the lattice [17].

In the domain of materials science, phonons are instrumental in dictating the thermal and dynamic behaviors of materials [33]. First principles phonon calculations, for instance, have been widely applied to predict material properties, highlighting the significance of phonons in materials research [51]. Such calculations aid in understanding how phonons contribute to the thermal conductivity and electrical properties of materials, enabling the design of materials with desired thermal and electronic characteristics. According to quantum mechanics, microscopic vibrations (sound waves) in solid media are quantized. This means that vibration energy can only be exchanged in the form of so-called phonons [43], which

have an energy which is Planck's constant multiplied by the phonon frequency. The energy of each phonon is given by: $E = \hbar\,\omega$, where ω is the angular frequency and $\hbar$ is the reduced Planck's constant.

An understanding of lattice excitations (phonons), is essential for comprehending, forecasting, and controlling the characteristics of a material. Phonon dispersion relations are useful for calculating the heat capacity, vibrational entropy, and thermal conductivity of a material, as well as determining its mechanical stability.

1.3.3 Iron

The utilization of iron by humans may be traced back around 5,000 years [56]. Iron is an abundant substance in the cosmos, present in several stars [10], including our own sun [26]. Iron is the second most abundant metal element and the fourth most plentiful element in the earth's crust [13]. It makes up approximately 5% of the crust's weight and is thought to be the primary constituent of the earth's core [11]. Iron is present in the soil [34] in small amounts and can be found dissolved in groundwater [52] and the ocean [55] to a limited degree. Iron is seldom found in its pure form in nature [19], except in meteorites. It plays a diverse and important function in various fields, including geophysics, metallurgy, chemistry, and biology.

Iron is classified chemically as a transition metal, situated in period 4 of the periodic table, flanked by manganese to its left and cobalt to its right. It occupies the first position in group 8, previously known as group 8B, in the periodic table [12, 54]. Notably, iron is characterized by its ability to adopt multiple oxidation states that differ by single-electron steps, which is a hallmark of its versatile chemistry. This property significantly enriches its coordination and organometallic chemistry, allowing for a wide range of compounds with varied applications.

Iron, in its metallic form, embodies a spectrum of physics that is not only captivating but also foundational to geophysics and critical to the field of metallurgy. Its polymorphic nature [41], which manifests under variations in temperature, pressure, and alloying,

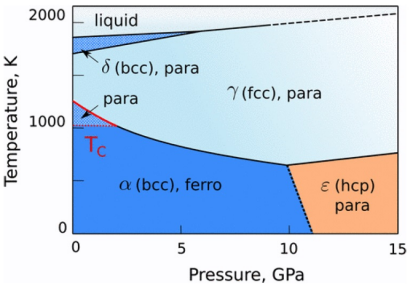


Figure 1.4: A portion of iron phase diagram

adds to its intrigue and utility. The phase diagram of iron is a fundamental aspect of its physical chemistry, illustrating how iron's structural phases vary with temperature and pressure (Fig 1.4). Iron is known to exist in three allotropic forms: alpha (α, ferrite) with a body-centered cubic (bcc) structure, gamma (γ, austenite) with a face-centered cubic (fcc) structure, and delta (δ) which also has a bcc structure, occurring at high temperatures [3]. The transitions between these phases are crucial for understanding the behavior of iron under various conditions, particularly in the formation of steel and in geophysical contexts. These transitions are not merely academic; they significantly influence iron's magnetic and mechanical properties also, which are crucial for its applications in technology and industry. For instance, the magnetic properties of iron, which are essential for its role in electrical engineering and electronics, vary significantly with its crystal structure. Similarly, the mechanical properties of iron, fundamental to its use in construction and manufacturing, are also deeply affected by its structural phase [39]. Understanding these properties and the conditions under which they change is vital for leveraging iron in various applications, from the core of our planet to the core of our technology.

Mechanical stability in materials, such as iron, relates to their ability to maintain structural integrity under mechanical stresses like tension, compression, and shear. Iron's mechanical stability is well-documented in the literature, often attributed to its high tensile strength [35] and durability [46]. On the other hand, iron's thermodynamic stability is influenced by its thermodynamic properties such as entropy, enthalpy, and Gibbs free energy [53].

Thermodynamic stability is concerned with the energy state of a material and its tendency to remain in a particular chemical or structural form rather than transform into a different form. A material is considered thermodynamically stable[44] if it is in the lowest possible energy state under given conditions, making it less likely to react or change structurally.

1.4 Methodology

The methodology of this study involves a sophisticated integration of computational techniques and innovative applications of genetic algorithms to optimize phonon dispersion models.

The study begins by establishing a body-centered cubic (BCC) structure for iron in python, setting the lattice parameters specifically at 2.86 Å, which is typical for iron. This step is fundamental as it defines the basic framework on which the phonon dispersion analysis is conducted.

Employing Phonopy, a powerful open-source software package, for Phonon Dispersion Analysis is utilized to carry out phonon dispersion calculations. Phonopy is advantageous due to its ability to integrate with multiple density functional theory (DFT) programs, allowing for accurate calculations of phonon band structures, density of states, and other thermal properties under constant volume and pressure conditions.

The study leverages experimental data from the supplemental materials of the refrence [28] to input initial force constants within the Phonopy software, focusing on configurations where BCC iron is known to be stable. This input serves as the baseline for further optimizations.

A genetic algorithm (GA) is implemented to optimize the force constants used in the Phonopy and iteratively adjusts these force constants to optimize the objective function. The algorithm includes force constants for the Born-von Kármán (BvK) fit for the zeroth and first nearest neighbors. The algorithm adjusts these parameters while keeping higher order constants fixed, focusing on enhancing the stability of the crystal under study. The

introduction of the root mean square error (RMSE) of negative phonon frequencies provides a quantitative assessment of the model's accuracy. By targeting the minimization of RMSE, the study ensures that the adjustments in the force constants effectively reduce the occurrence of imaginary phonon frequencies, thus predicting more stable configurations.The GA allows for continuous feedback and refinement of the force constants. This iterative process is key to approaching an optimal set of parameters that define a stable BCC iron structure under the modeled conditions.

The regions of stability (pockets where the crystal remains mechanically stable) in the high symmetry space are identified through the avoidance of negative phonon dispersion. These regions are critical for understanding the conditions under which BCC iron can maintain its structural integrity under various temperatures and pressures.

This methodological approach not only enhances the understanding of BCC iron's mechanical stability but also sets a precedent for using evolutionary algorithms in materials science to optimize complex computational models. The integration of experimental data with advanced computational techniques represents a significant advancement in the study of material stability, providing a robust framework for future explorations into other materials and conditions.

Chapter 2

Theoretical Framework

2.1 Born-von Kármán (BvK) Model

The Born-von Kármán model for crystal structures provides a sophisticated framework for understanding the vibrational properties and force constants in crystals. It is integral in the study of lattice dynamics, can offer insights into how atomic interactions and crystal symmetries affect the mechanical and thermal properties of materials.[59]
Research has extended the application of the Born-von Karman model [42] to complex crystal structures, analyzing how these structures accommodate various types of lattice vibrations [25] and the implications for material properties [9].
In crystals, it is presumed that atoms are connected by massless springs [22] providing a restoring force against displacements and they move around their equilibrium positions $\vec{r_{l\kappa}}$ with displacements $\vec{u_{l\kappa}}$, where l and κ are the labels of unit cells and atoms in each unit cell, respectively. If $\vec{R^a_{l\kappa}}$ is the instantaneous position of the κth atom in the lth unit cell in the direction of a, then

$$\vec{R^a_{l\kappa}} = \vec{r^a_{l\kappa}} + \vec{u^a_{l\kappa}} \tag{2.1}$$

Crystal potential energy Φ is presumed to be an analytic function of the displacements of the all atoms in the crystal. The Taylor expansion of the potential energy about $\vec{u^a_{l\kappa}} = 0$, i.e., for the case of equilibrium positions,

$$\Phi = \Phi_0 + \sum \Phi^a_{l\kappa} + \frac{1}{2} \sum_{al\kappa} \sum_{bl'\kappa'} \Phi^{ab}_{l\kappa l'\kappa'} u^a_{l\kappa} u^b_{l'\kappa'} + \dots \tag{2.2}$$

where orthogonal directions are indexed by a, b, c, ... and the coefficients are the derivatives of the potential with respect to atom displacements:

$$\left.\begin{array}{rcl} \Phi^a_{l\kappa} & = & \frac{\partial \Phi}{\partial u^a_{l\kappa}}\Big|_{u^a_{l\kappa}=0}; \\ \Phi^{ab}_{l\kappa l'\kappa'} & = & \frac{\partial^2 \Phi}{\partial u^a_{l\kappa}\partial u^b_{l'\kappa'}}\Big|_{u^a_{l\kappa}=0,\ u^b_{l'\kappa'}=0}; \\ \Phi^{abc}_{l\kappa l'\kappa' l''\kappa''} & = & \frac{\partial^3 \Phi}{\partial u^a_{l\kappa}\partial u^b_{l'\kappa'}}\partial u^c_{l''\kappa''}\Big|_{u^a_{l\kappa}=0,\ u^b_{l'\kappa'}=0,\ u^c_{l''\kappa''}=0}; \\ \ldots\ \ldots\ \ldots\ \ldots\ \ldots & & \end{array}\right\} \tag{2.3}$$

With small displacements at constant volume, the problem of atomic vibrations is solved with the second-order terms as the harmonic approximation, and the higher order terms are treated by the perturbation theory. Crystal symmetry is used to increase the numerical accuracy of force constants and lower computing costs.[51] The solutions to the equations of motion then have the form of planewaves with wavevector $\vec{q}$, angular frequency $\omega_{\vec{q}j}$ and polarization $\vec{e}_{\vec{q}j}$. Then the dynamics of any crystal structure can be reduced to an eigenvalue problem,

$$\tilde{D}(\mathbf{q})\mathbf{e}_{\mathbf{q}j} = \omega^2_{\mathbf{q}j}\mathbf{e}_{\mathbf{q}j} \tag{2.4}$$

where j is the band index and the elements of the dynamical matrix $\tilde{D}(\mathbf{q})$ are the submatrices $\tilde{D}_{\kappa\kappa'}(\mathbf{q})$, which are the Fourier transforms of force constant matrices $\Phi_{l\kappa l'\kappa'}$, and all the polarization vectors have been placed into a single vector $\mathbf{e}_{\mathbf{q}j}$.

2.2 Stability condition

In the harmonic approximation, the stability condition requires that all phonons have real and positive frequencies [15].This is equivalent to the condition that the second derivative of the potential energy with respect to atomic displacements is greater than zero ($\frac{\partial^2 \Phi}{\partial u^a_{l\kappa}\partial u^b_{l'\kappa'}} > 0$)[51] which indicates a local minimum in the potential energy. In this case, the equilibrium

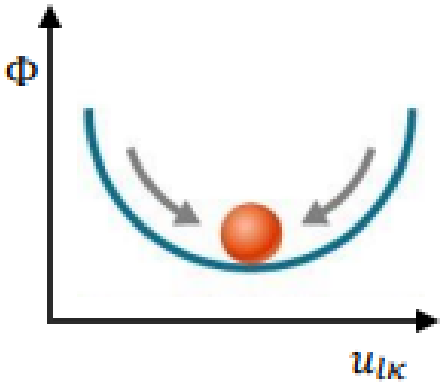


Figure 2.1: Stable equilibrium

position is considered stable (Fig: 2.1) because any small displacement from this point results in an increase in potential energy, leading the system to return to equilibrium.

Any appearance of negative frequencies or imaginary modes in the phonon dispersion curves indicates potential instability regions within the crystal lattice. These instabilities suggest that under certain virtual thermodynamic conditions, such as changes in volume or external pressure, the system might exhibit dynamic instability, leading to phase transitions or alterations in mechanical properties [51].

Chapter 3

Computational Framework

3.1 Phonopy

Phonopy, an open-source software package, provides a robust set of tools for phonon calculations at both harmonic and quasi-harmonic levels [49]. Its flexibility across various DFT software enhances its utility in calculating phonon band structure, density of states (DOS), and partial DOS, along with thermal properties [5] under constant volume conditions such as free energy, entropy, and heat capacity. Additionally, by employing quasi-harmonic approximations, Phonopy can also predict properties under constant pressure scenarios, such as isobaric heat capacity and thermal expansion coefficients. This makes Phonopy a comprehensive tool for materials science researchers interested in the vibrational properties of materials [50].

Phonopy utilizes a direct force-constant method that leverages finite displacements and symmetry considerations to compute elements of the dynamical matrix, crucial for accurate phonon calculations [57]. The compatibility with various DFT programs like VASP and Abinit, among others, ensures that Phonopy is versatile and widely applicable in materials research. It aids in the exploration of phonon properties in a variety of materials, further facilitating the investigation of their thermomechanical properties. This integration of different computational methods within Phonopy not only broadens its applicative spectrum in condensed matter physics but also highlights its role in advancing computational materials science [50].

3.1.1 Phonopy work flow

The workflow of Phonopy typically involves two stages (Fig: 3.1), indicating a sequential process where the "Phonopy pre-process" is the initial step followed by the "Phonopy post-process."

Phonopy pre-process: In this stage, Phonopy utilizes the crystal structure which includes the unit cell and supercell size to create the supercell, which is a larger, periodic replication of the unit cell. There are two main pathways to calculate force constants between atoms in the supercell:
(1) Atomic Forces from Finite Displacements: This method involves computing atomic forces when atoms are slightly displaced from their equilibrium positions. The displacement generates forces on the atoms, which are then used by Phonopy to calculate force constants.
(2) Given Force Constants: In this method, the force constants are directly provided (perhaps calculated from another software or method). Phonopy uses these constants to compute the phonon properties without the need for initial atomic displacements.

Phonopy post-process: In this stage, Phonopy takes the computed or provided force constants and processes these data to derive the phonon properties of the material. This stage involves calculating the phonon frequencies, generating dispersion relations, and producing density of states diagrams, among other properties.

3.1.2 Phonopy input and output files

Phonopy requires specific input files to perform phonon calculations. These files contain necessary information about the crystal structure, the computational parameters, and the details for interfacing with external force calculation software. Phonopy typically uses a structure file in a format compatible with various calculators, like the VASP POSCAR

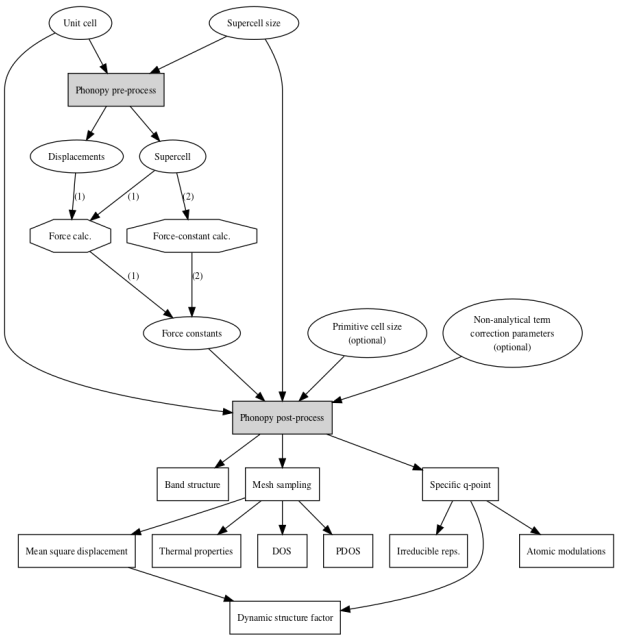


Figure 3.1: Phonopy work flow

format. This format includes details such as lattice parameters, the number of each type of atom, and their positions in either direct that the atomic positions are represented in fractional (reduced) coordinates or Cartesian coordinates. Another important input file is Phonopy configuration file (name.conf) which contains settings and parameters directing the phonon calculation processes. This file is loaded into Phonopy with a command like $ phonopy name.conf, allowing users to customize their computational workflow.

Phonopy generates several output files such as phonopy.yaml and phonopy_disp.yaml, which store detailed information about the crystal structure, including primitive and supercell configurations, and interface settings for the calculators used. The phonopy.yaml file can store the results of phonon calculations, such as force sets, Born effective charges, and force constants. Phonopy can also generate PDF files of phonon band structures, which visually represent the phonon dispersion relations as a function of wave vector along various directions in the crystal lattice. This visualization is essential for understanding the dynamics of lattice vibrations and their impact on material properties such as thermal conductivity and elastic properties.

3.2 Genetic Algorithm

Evolutionary algorithms (EAs) are a subset of evolutionary computation inspired by biological evolution principles [38, 32] such as reproduction, mutation, recombination, and selection. These algorithms are used in problem-solving and optimization processes across various domains [1]. Genetic Algorithms, Evolution Strategies, Evolutionary Programming, Genetic Programming, Learning Classifier Systems, Differential Evolution are popular types of EAs. Genetic algorith is the most common used EA that particularly mimic the process of natural selection where the fittest individuals are selected for reproduction to produce offspring of the next generation.

Genetic algorithms operate on a population of potential solutions applying the principle of survival of the fittest to produce increasingly better approximations to a solution. At each generation, a new set of approximations is created by the process of selecting individuals according to their level of fitness in the problem domain and breeding them together using operators borrowed from natural genetics [23]. This process leads to the evolution of populations of individuals that are better suited to their environment than the individuals that they are derived from, provided with robust solutions to optimization and search problems [7].

Genetic algorithms have been successfully applied in various fields including but not limited to optimization, automatic programming, machine learning, economics, immune systems, ecology, population genetics, and learning classifier systems. In particular, the use of GAs in optimizing the parameters of a cogeneration system demonstrated significant improvements in thermodynamic models [2]. Moreover, the application in multi-objective problems like the NSGA-II, an elitist multi-objective genetic algorithm, offers a method for optimizing a variety of conflicting objectives [6].

Recent developments in GAs include adaptations that integrate with other optimization techniques to address more complex problems such as dynamic scheduling and multi-modal optimization. For example, the integration of GAs with machine learning techniques has

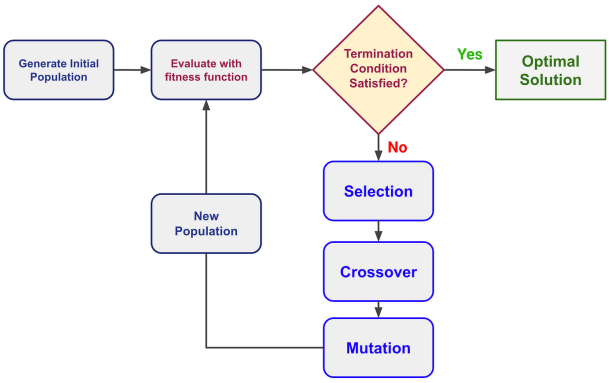


Figure 3.2: Core Cycle of GAs

improved the prediction accuracy in applications like wind speed forecasting [24]. Furthermore, hybrid approaches combining GAs with other heuristic algorithms have shown improved performance in production scheduling [58].

In conclusion, genetic algorithms are a powerful tool in the arsenal of computational intelligence, providing robust solutions across a wide range of complex problem domains. As computational capabilities grow, the potential applications of genetic algorithms continue to expand, offering vast opportunities for both theoretical advancements and practical implementations in various scientific and engineering fields.

3.2.1 Common Cycle of Genetic Algorithms

The five phases of a genetic algorithm (Fig: 3.2) form the core cycle through which a GA evolves solution to optimization problems. Here's a detailed description of each phase:

Initial Population

The initial population is the starting point of a genetic algorithm. It consists of a set of potential solutions to the given problem, represented as chromosomes. Each chromosome encodes candidate solutions as strings of genes (Fig: 3.3) , which can be binary, alphanumeric, or more complex structures depending on the problem domain. The initial population is typically generated randomly to cover a broad area of the search space.

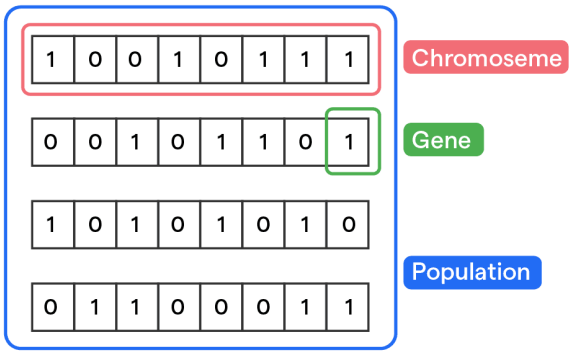


Figure 3.3: Initial population

Generating a diverse initial population helps in effectively exploring different regions of the search space [1].

Fitness Function

The fitness function evaluates how close a given solution is to fulfilling the set objectives and constraints of the specific problem. This function plays a critical role as it directly influences the selection process by determining which solutions are superior and thus more likely to reproduce. The design of the fitness function significantly affects the GA's efficiency and ability to locate the global optimum. In many cases, the fitness function is problem-specific and must be defined carefully to ensure that it guides the evolutionary process toward the optimal solution [2].

Selection

Selection is the stage in a GA where individual solutions are chosen from the current population to breed a new generation. Selection is based on the principle of survival of the fittest. Individuals with higher fitness are more likely to be selected for reproduction. Common selection methods include roulette-wheel selection, tournament selection, and rank selection. This phase is crucial as it focuses on exploiting the best solutions and is responsible for sending good genetic material to the next generation, thus ensuring the

"survival of the fittest" [18].

Crossover

Crossover, or recombination, is a genetic operator used to combine the genetic information of two parents to generate new offspring. It is one way GAs create a new generation of populations. Crossover occurs during reproduction and is intended to allow beneficial traits from two different individuals to be combined, potentially producing more viable solutions in the new generation. Techniques like single-point crossover, multi-point crossover, and uniform crossover vary in how and where the genetic material is combined [6].

Mutation

Mutation is an operator used to maintain genetic diversity from one generation of a population of genetic algorithm solutions to the next. It is analogous to biological mutation. The purpose of mutation in GAs is to allow the algorithm to avoid local minima by preventing the population from becoming too similar to each other, thus maintaining diversity within the population and enabling the discovery of new solutions. Mutation typically occurs at a low probability rate and involves altering one or more gene values in a chromosome from its initial state. This can result in entirely new gene values being introduced into the gene pool [47].

Together, these phases create a loop that drives the search towards increasingly better solutions by mimicking the process of natural evolution. This iterative process repeats until a termination condition is met, such as a maximum number of generations or a satisfactory fitness level.

In addition, the elitism technique, the best individuals (or a few of the best individuals) from each generation are carried over to the next generation unchanged, is used to prevent loss of the best-found solutions due to crossover and mutation operations. It can significantly affect the performance and convergence speed of the evolutionary process. Including elitism

helps to preserve good genetic material and accelerates the convergence of the algorithm towards an optimal solution.

The primary benefit of using elitism in a genetic algorithm is the assurance that the quality of the solution does not degrade over generations, as the best solutions are always preserved. This is particularly useful in scenarios where the goal is to not only find a good solution but to ensure that the solution quality consistently improves or remains at the highest discovered quality [18].

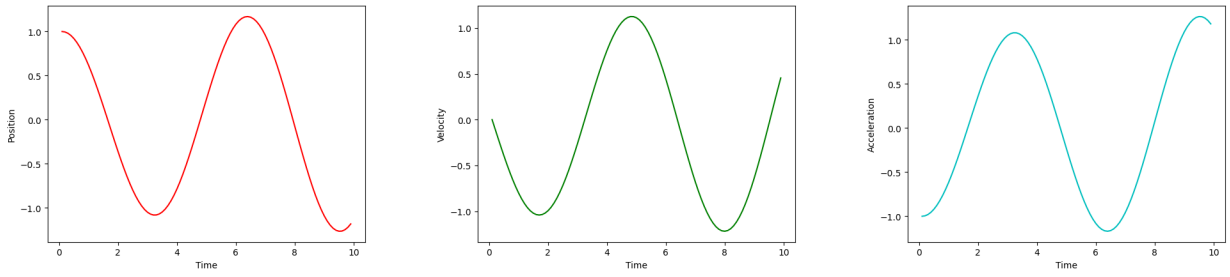
Chapter 4

Discussion and Results

4.1 Work done in Fall-2022

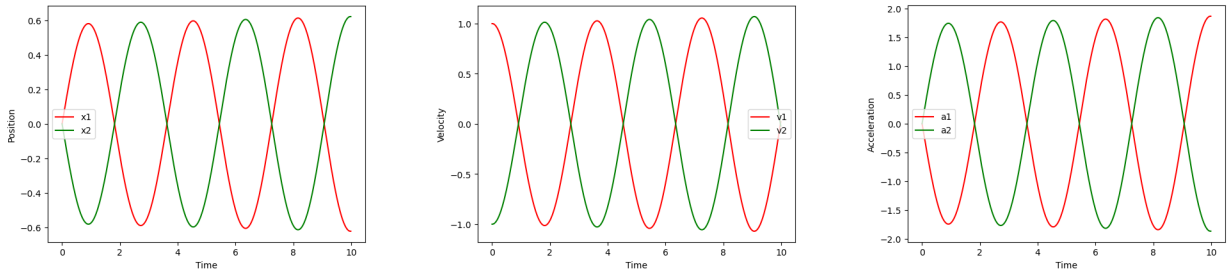
At the very , we developed a Python script simulates molecular dynamics for one mass and one spring on google colab by initializing variables for position, velocity, acceleration and time, with predefined constants for mass and force constant and time step. It runs a simulation loop for certain iterations where it updates these variables using basic Hooke's law and Newton's second law. The program stores the time, position, velocity, and acceleration values in lists, which are then plotted using matplotlib to display how each of these variables changes over the course of the simulation. The resulting graphs (Fig:4.1) show the evolution of position, velocity, and acceleration as functions of time, providing visual insights into the dynamics of the system.

We updated the model with a more intricate physical scenario involving two masses connected by three springs, instead of just one mass and spring. In the simulation, both



(a) Position vs Time (b) Velocity vs Time (c) Acceleration vs Time

Figure 4.1: Dynamics of a single mass



(a) Position vs Time (b) Velocity vs Time (c) Acceleration vs Time

Figure 4.2: Dynamics of two masses

masses are assigned an identical mass of 1.0 kg and the springs connecting them have a uniform force constant of 1.0 kg/s^2, ensuring symmetry in the dynamic interactions and simplifications in the mathematical model of the system. In the new script, we adopted NumPy array in lieu of python list. Because, NumPy array is more memory efficient than list, and provides a wide range of mathematical functions that are optimized for array operations [29], reducing the need to implement such functions manually and ensuring they run faster than if they were implemented on lists using Python loops. The advancement in the new program not only provides a more realistic simulation of physical systems (like coupled oscillators) but also serves as a better computational tool for understanding more complex dynamics in physics. The results are depicted graphically in the (Fig: 4.2) for each mass's position, velocity, and acceleration, enhancing the analysis of the system's dynamics.

Link for the complete programs:

1. Click https://colab.research.google.com/drive/13xu5PFwMwXNSgYMOd6pRHvSWpvhUBNBu?us
   for single mass.

2. Click https://colab.research.google.com/drive/13xu5PFwMwXNSgYMOd6pRHvSWpvhUBNBu?us
   for two masses.

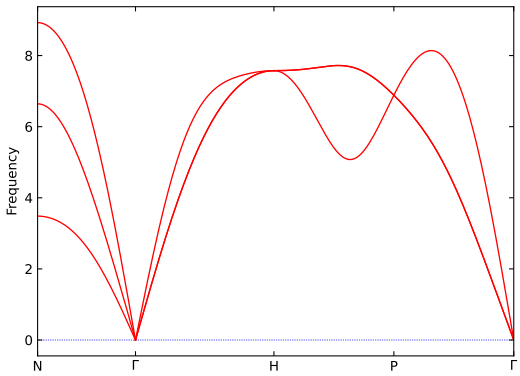
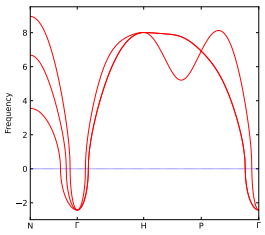


Figure 4.3: Phonon band for BCC iron

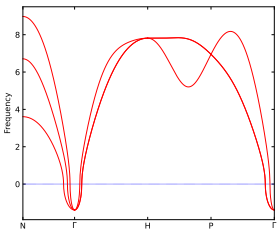
4.2 Work done in Spring-2022

A Python script was designed for simulating the force constants in a crystal lattice structure and generating associated phonon band structures using the Phonopy software package. The script begins by defining several variables like the root directory, lattice parameter, number of atoms etc. Ideal positions of atoms in a BCC lattice structure was read from a predefined file using NumPy.genfromtxt(filename) command and processes it to determine the ideal interatomic distances by applying minimum image conventions (mic). This is crucial for distinguishing between different types of neighbors based on their distances.

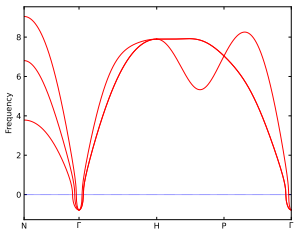
The main computational part of the script involves calculating the phonon dispersion using Phonopy. In the BvK model, there are 14 parameters (force constant) up to fifth nearest neighbor. Among them 13 parameters from first to fifth nearest neighbor are collected from the supplementary resources of the reference [28] and the zeroth nearest neighbor force constant was computed using the condition that suppercell has no over all translation. Once the force constants matrix is fully populated, the script writes this data to a format compatible with Phonopy to generate phonon band structure and related outputs. The result of the program is shown in (Fig: 4.3).



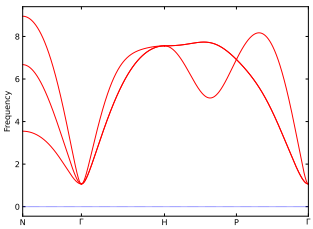
(a) $\alpha_0 = 9.362, \alpha_1 = -0.95$



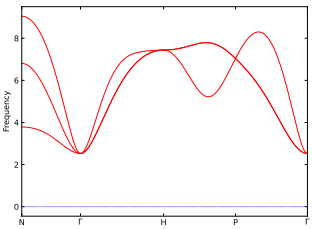
(b) $\alpha_0 = 9.462, \alpha_1 = -0.85$



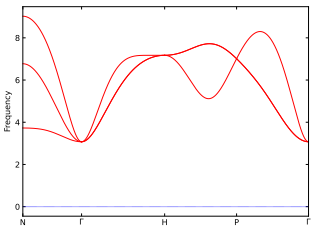
(c) $\alpha_0 = 9.762, \alpha_1 = -0.85$



(d) $\alpha_0 = 9.362, \alpha_1 = -0.75$



(e) $\alpha_0 = 9.762, \alpha_1 = -0.65$



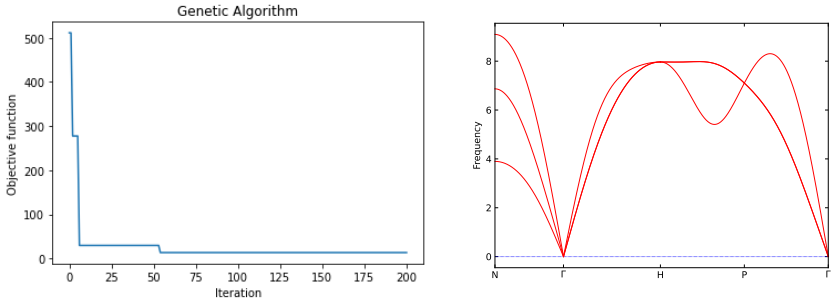
(f) $\alpha_0 = 9.662, \alpha_1 = -0.55$

Figure 4.4: Phonon dispersion results

4.3 Work done in Summer-23, Fall-24 and Spring-24 on GA

We seek to find the range of the force constant for the BvK model fit. We have tried to find some values blending the first two parameters, developing a new program where the value of the first parameter was increased by 0.1 and the value of the second parameter decreased by 0.1. It proved quite impossible to get a set of values that fit the BvK model for a stable crystal. Some of the results are exemplified in the (Fig: 4.4).

So, this gives a great motivation for us to apply the evolutionary algorithm in our program to get a set of parameter values for BvK model fit. In developing a genetic algorithm (GA), we employed the open source package, Phonopy, known for its robust calculation of phonon properties. The GA initiates with two distinct sets of initial values for two parameters which are taken randomly from two interval of real numbers. The objective function for the GA is defined as the root mean square error (RMSE) of the



(a) Value of objective function for 200 generations

(b) Population size = 10, Generation = 200

Figure 4.5: Output from GA

phonon frequencies, incorporating penalties that account for physical constraints of the system. As the GA progresses through numerous generations, there is a clear convergence of parameter values (Fig: 4.5) towards those that more accurately reflect the phonon dispersion observed in BCC iron. This convergence demonstrates the utility of evolutionary algorithms in complex parameter optimization tasks in materials science.

This methodology exemplifies the application of evolutionary computation principles—such as selection, mutation, and reproduction—to effectively solve problems in physical sciences, specifically in the optimization of model parameters based on experimental data.

4.4 Proof of concept

This methodology exemplifies the application of evolutionary computation principles—such as selection, mutation, and reproduction—to effectively solve problems in physical sciences, specifically in the optimization of model parameters based on experimental data.

Chapter 5

Proposal

5.1 Introduction

Body-centered cubic (BCC) iron shows significant potential for diverse applications due to its inherent mechanical and magnetic properties. Understanding its stability under different conditions is crucial for advancements in metallurgy and materials science. Present works have used phonon dispersion analysis to study vibrational properties and lattice dynamics. This proposal aims to build on these foundations by optimizing the computational models further using evolutionary algorithms.

5.2 Objective

The primary objective of this research is to extend and optimize a genetic algorithm for predicting the mechanical stability of body-centered cubic (BCC) iron within the Born-von Kármán (BvK) parameter space under various environmental conditions, focusing on temperature and pressure impacts. This research aims to expand on previous investigations into the mechanical stability of BCC iron, focusing on its behavior under various conditions in the Born-von Kármán (BvK) parameter space. We have two specific objectives-

Objective 1:

Extend and optimize the genetic algorithm to explore and identify stability regions in BvK parameter space for BCC iron. Reinforcement Learning (RL) can be used to dynamically

adjust the genetic algorithm's parameters (e.g., mutation rate, crossover probability) in response to its performance. By modeling the parameter tuning process as a reinforcement learning problem, where the agent's actions are the adjustments to the genetic algorithm parameters and the rewards are based on improvements in finding stability regions, the genetic algorithm can become more efficient over time.

Objective 2:

Generalize the model to other BCC metals like Vanadium (V), Niobium (Nb), Tantalum (Ta), and Chromium (Cr) to investigate commonalities and variances in stability regions across different BCC metals.

Based on these two main objectives, we will write up peer-reviewed publications detailing the findings and methodologies, enhancing the visibility and impact of the research.

5.3 Methodology

Genetic Algorithm Development:

- Extend the current genetic algorithm to handle five BvK parameters.
- Implement parallel processing to enhance the computation speed.
- Adapt the algorithm to dynamically adjust based on real-time simulation feedback, focusing on stability regions within the BvK parameter space.

Simulation and Data Analysis:

- Generalize the algorithm to handle arbitrary volumes and force constants, and validate the model with BCC metals, focusing on phonon dispersion analysis.
- Utilize the modified genetic algorithm to find optimal BvK parameters that align with the experimental and simulated data.

		Summer 2024	Fall 2024	Spring 2025	Summer 2025	Fall 2025	Spring 2026
Objective 1 : determine region of stability of BCC Fe in BvK parameter space	Extend genetic algorithm code to 5 BvK parameters						
	Parallelize code						
	Find new sets of. constraints that produce hypervolumes in BvK parameters space						
	Write paper on Fe						
Objective 2 : determine region of stability of arbitrary BCC crystals in BvK parameter space	Generalize genetic algorithm code to arbitrary volumes and force constants						
	Test generalized GA with several BCC metals (V, Nb, Ta, Cr)						
	Write paper on generalized GA						
	Write dissertation						

Figure 5.1: Timeline

Testing and Validation:

Test the generalized genetic algorithm across multiple BCC metals like Vanadium (V), Niobium (Nb), Tantalum (Ta), and Chromium (Cr) to validate its applicability and robustness. Compare the algorithm's predictions with existing experimental data for validation. Machine learning regression models can be employed to validate these predictions against existing experimental data. Such models can quantify the accuracy and reliability of the genetic algorithm's outputs and suggest areas for refinement.

5.4 Expected Outcomes

- Development of a more robust and versatile genetic algorithm capable of exploring complex parameter spaces.
- Comprehensive mapping of stability regions for BCC iron and other metals, contributing valuable data to materials science.

5.5 Timeline for the futer works

The (Fig: 5.1) shows the tentative timeline to accomplish the work.

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Vita

My name is Amir Husen, and I am a doctoral candidate in Computational Science at the University of Texas at El Paso, supervised by Dr. Jorge A. Munoz. Prior to this, I spent thirteen years teaching at Northern University Bangladesh and Sonargaon University in Dhaka, covering departments such as Business Administration, Mechanical Engineering, and Naval Architecture and Marine Engineering. I also coordinated undergraduate programs in Naval Architecture and Marine Engineering.

My academic background in mathematics has driven my appreciation for computational tools to solve complex scientific challenges. During my undergraduate years, I learned programming languages like C, FORTRAN, and MATHEMATICA, which laid the foundation for my current pursuits. Now in my fourth semester of the Ph.D. program, I have studied Introduction to Computational Science, Advanced Scientific Computing, and Mathematical and Computational Modeling, Machine Learning along with others. I applied my computational skills in a Machine Learning project by developing an image classification model using a Convolutional Neural Network (CNN), which demonstrated my ability to apply theoretical knowledge practically. As a research assistant, I spearheaded a Python-based Molecular Dynamics simulation project, utilizing the 'Phonopy' package and an evolutionary algorithm to analyze phonon dispersion and explore Born-von Kármán force constants, thereby enhancing our understanding of crystal lattice vibrations and stability.

Looking forward, I aim to merge my skills in Mathematics, Computational Science, and programming to become a leading researcher in fields like Artificial Intelligence, Cyber Security etc.

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