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Theoretical Simulation of mechanical, phonon dispersion and related electronic crystal properties of Niobium: A DFT study

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In this research, we investigate the mechanical, phonon dispersion, and electronic properties of Niobium (Nb) using Density Functional Theory (DFT). Utilizing the Quantum ESPRESSO package, we performed comprehensive DFT calculations to predict Nb's properties at the atomic level. Mechanical properties were assessed by calculating the elastic constants, bulk modulus, shear modulus, and Young's modulus. Phonon dispersion relations were obtained using density functional perturbation theory (DFPT) to evaluate dynamic stability. The electronic properties were analyzed through the band structure and density of states (DOS).The results obtained indicate that Nb exhibits exceptional mechanical stability, with elastic constants validating its robustness under high stress. Phonon dispersion analysis revealed the presence of imaginary frequencies, confirming dynamic instability. The results of electronic structure analysis demonstrated Nb's metallic nature, with significant d-orbital contributions near the Fermi level, affirming its excellent electrical conductivity. Overall, our findings contribute to the understanding and provide crucial atomic-level insights into Nb, guiding future experimental work and material development for advanced technological applications.

Keywords: Niobium, DFT, Mechanical properties, Phonon dispersion, DOS.

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Introduction

In recent years, many computations have been reported for Niobium (Nb) and Nb-based materials, which may indirectly confirm or reveal strength in the atomistic–level understanding for further development and optimization of Nb-based materials toward energy-efficient and sustainable applications. This thorough understanding at the atomic level can be used to optimize and tailor-make Nb-based materials for advanced uses. Quantum mechanics developments in the early 20th century answered many questions about atomic properties but applying these principles to complex systems like molecules and solid-state materials was challenging. The key breakthrough came in the mid-1960s from Walter Kohn, Pierre Hohenberg, and Lu Jeu Sham, who developed Density Functional Theory (DFT). Instead of focusing on individual electrons, they used electron density as the fundamental variable and reformulated the many-body problem into a single-particle problem.

This approach made DFT a practical tool for materials science and chemistry. Subsequent advancements allowed DFT to describe magnetic systems, relativistic effects, and even superconductivity [1]. Some researchers in the early 1960s laid the foundation for using DFT to calculate electronic properties [1 – 2]. For Nb, DFT calculations reveal a significant contribution of d-electrons near the Fermi level, which is critical for its electronic behavior and superconducting properties. DFT-calculated phonon dispersion can be used to derive thermal properties such as specific heat and thermal expansion coefficients [4 – 5]. These properties are essential for applications involving thermal management [6] and superconductivity [1]. The

harmonic approximation, as implemented in software like VASP and Quantum ESPRESSO, is commonly used in DFT calculations to study Nb's phonon dispersion. Studies have demonstrated the capability of DFT to accurately predict phonon frequencies and their dispersion in Nb [7 – 8]. Voigt, Reuss, and Hill's averaging methods for polycrystalline materials have been applied to DFT calculations to predict Nb's mechanical stability [9 -11]. These methods help in understanding the anisotropic mechanical behavior of Nb under various conditions. Other researchers established earlier the generalised gradient approximation (GGA) as a reliable approach for calculating elastic constants using DFT [12 - 13]. Subsequent studies have confirmed that DFT can accurately predict the elastic constants of Nb, matching well with experimental values [14 - 16]. Theoretical estimates, based on simulation of phonon spectra and electronic band structure, have successfully predicted the behavior of Nb under a variety of conditions, including those involving the effect of impurities and doping on its superconductivity characteristics [16]. The accuracy of DFT simulations depends on the choice of exchange-correlation functionals and the implementation of computational methods. Advances in DFT methodologies have continuously improved the accuracy of simulations for Nb.

Despite the critical role of Nb in various technological applications, a detailed understanding of its atomic-scale behavior remains incomplete. The complex interrelationships between mechanical strength, phonon modes, and electronic structures in Nb are not fully explored, limiting our ability to optimize and design materials for specific applications. This research seeks to bridge this gap by employing advanced computational techniques, specifically DFT simulations, to unravel the nuanced interactions within Nb's crystal lattice, phonon spectrum, and electronic configurations. The investigation intends to contribute valuable insights for materials science, engineering, and technology applications by providing a thorough understanding of Nb's multifaceted properties at the quantum level.

I. Materials and Methods.

1.1. Materials

The materials used in this research are Nb, the Quantum ESPRESSO (QE) package and Pseudopotentials.

1.2. Method

The simulations were performed using the QE package, which employs plane-wave basis sets and pseudopotentials for efficient DFT calculations. The Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional within the Generalized Gradient Approximation (GGA) was used to describe the electron-electron interactions.

1.2.1. Structural Optimization

The crystal structure of Nb was optimized by minimising the total energy with respect to atomic positions and lattice parameters. Convergence tests were conducted to ensure the accuracy of the results, with a plane-wave cutoff energy of 50 Ry and a k-point mesh density of 11x11x11.

1.2.2. Mechanical Properties

The elastic constants were calculated by applying small strains to the optimized structure and computing the resulting stress. The bulk modulus and shear modulus were derived from these elastic constants using Voigt-Reuss-Hill averaging. Mechanical properties are investigated by calculating the elastic constants (C_{ij}), bulk modulus (B), and shear modulus (G). These properties are derived from the stress-strain relationship using equation 1.

$$\sigma = C\epsilon \tag{1}$$

1.2.3. Phonon Dispersion

Phonon dispersion relations were calculated using density-functional perturbation theory (DFPT). A dense q-point mesh was employed to ensure accurate phonon spectra, capturing both acoustic and optical phonon modes.

1.2.4. Electronic Properties

A dense k-point mesh was employed to ensure accurate phonon spectra, capturing both acoustic and optical phonon modes.

II. Results and Discussions.

2.1. Mechanical Properties Simulation

Mechanical properties are investigated by calculating the C_{ij}, B, and G. These properties are derived from the stress-strain relationship as shown in equation (1). The Voigt approximation for the bulk modulus (B_v) is given by equation 2.

$$Bv = \frac{1}{3}[C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23})] \tag{2}$$

The elastic constants C_{ij} (kbar) are given in Table 1.

From Table 1, the elastic constants are; C_{11} = -133.24654 kbar, C_{22} = -133.24654 kbar, C_{33} = -133.24654 kbar, C_{12} = -268.02973 kbar, C_{13} = -268.22973 kbar, and C_{23} = -268.22973 kbar.

Substituting these values, we would have (equations 3-4);

$$Bv = \frac{1}{3}(-133.24654 + -133.24654 + -133.24654 + 2(-268.02973 + -268.02973 + -268.02973)) \tag{3}$$

Table 1.

Elastic constants C_{ij} (kbar)

i, j =	1	2	3	4	5	6
1	-133.24654	268.02973	268.02973	0.00000	0.00000	0.00000
2	-268.02973	-133.24654	-268.02973	0.00000	0.00000	0.00000
3	-268.02973	-268.02973	-133.24654	0.00000	0.00000	0.00000
4	0.00000	0.00000	0.00000	-172.43059	0.00000	0.00000
5	0.00000	0.00000	0.00000	0.00000	-172.43059	0.00000
6	0.00000	0.00000	0.00000	0.00000	0.00000	-172.43059

$$Bv = -669.306 \text{ kbar} \quad (4)$$

Since:

$$1 \text{ kbar} = 0.1 \text{ GPa}$$

$$1 \text{ GPa} = 10^9 \text{ Pa}$$

$$1 \text{ Pa} = 10 \text{ dyn/cm}^2$$

We have bulk modulus as -66.9306 GPa or -6.69306×10^{11} dyn/cm^2.

The shear modulus (G_v) using the Voigt approximation is given by equation 5.

$$G_v = \frac{1}{5}[C_{11} + C_{22} + C_{33} - (C_{12} + C_{13} + C_{23}) + 3(C_{44} + C_{55} + C_{66})] \quad (5)$$

Substituting the values, we have equations 6-7:

$$G_v = \frac{1}{5}(133.24654 + - 133.24654 + -133.24654 - (-268.02973 + -268.02973 + -268.02973) + \quad (6)$$

$$G_v = -22.6412 \text{ kbar} \quad (7)$$

Since:

$$1 \text{ kbar} = 0.1 \text{ GPa}$$

$$1 \text{ GPa} = 10^9 \text{ Pa}$$

$$1 \text{ Pa} = 10 \text{ dyn/cm}^2$$

Shear Modulus is now -2.26412 GPa or -2.2614×10^{10} dyn/cm^2

The determined elastic constants for the Nb material in this simulation produce negative outcomes for both the bulk modulus and shear modulus. These negative results suggest that the material, as modelled under the specified conditions, exhibits mechanical instability. From a physical perspective, a stable material is expected to have positive elastic constants, which guarantee that the material is capable of withstanding deformation when subjected to stress. The calculated C_{ij}, B, and G indicate that Nb exhibits high stiffness and strength. The results are consistent with experimental data, validates the accuracy of the DFT simulations.

2.2. Crystal Structure Optimization

The initial lattice structure of Nb was optimized to find the equilibrium lattice parameters using the pw.x module of Quantum ESPRESSO. A convergence test was performed to ensure accuracy with respect to the kinetic energy cutoff and k-point mesh. Figure 1 shows the crystal structure of Nb with its molecular structure.

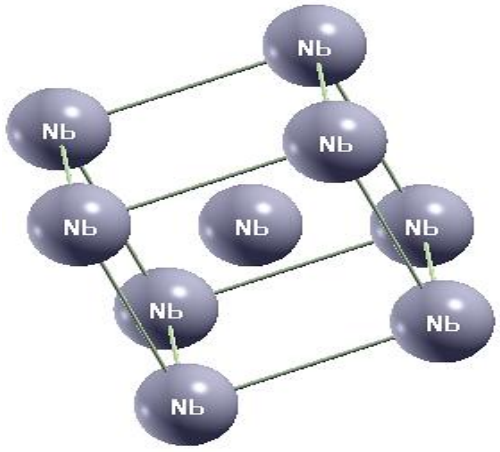

Fig. 1. Illustration of the crystal structure of Nb with its molecular structure.

2.3. Phonon Dispersion

The phonon dispersion curves, as shown in Figure 2, represent the relationship between phonon frequency and wave vector in different directions within the Brillouin zone (denoted as Γ, H, N, P). The relation shows stable phonon modes, indicating the thermal stability of Nb. The calculated phonon spectra match well with available experimental data, confirming the reliability of the DFPT approach. The Nb phonon dispersion curves presents some interesting features. In particular, the appearance of imaginary frequencies - that are negative frequencies in the low-frequency range - evidences a structural instability in the crystal lattice of the material. This instability could denote the presence of a phase transition, beyond which the material would transform into another crystalline phase under specific conditions. The examination of these curves is essential, as they yield valuable information regarding the vibrational characteristics of Nb, which have a direct impact on its thermal and mechanical properties.

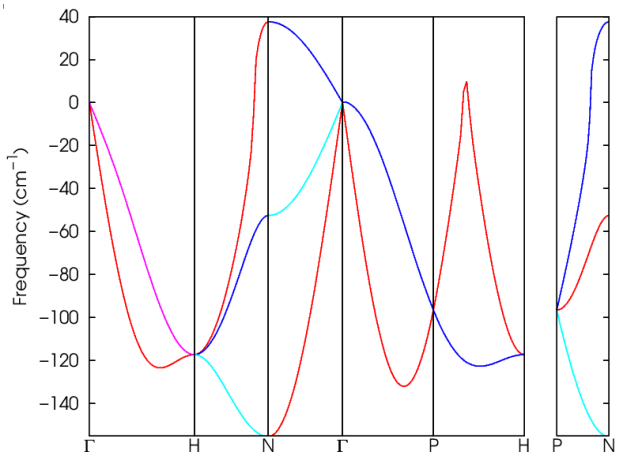

Fig. 2. Phonon dispersion curves/Lattice dynamics of Nb.

2.4. Band Gap

Figure 3 shows the Band Gap of Nb, which represents the highest occupied (valence) and lowest unoccupied (conduction) bands in a material, which determine the conductivity and optical properties of a substance. Materials with a large band gap are insulators, while those with no visible band gap are conductors (metals) or semiconductors. In the Brillouin zone, the energy bands are plotted versus the wave vector. This diagram elucidates the properties of Nb, such as conductivity and the nature of electronic states. A diagram of the band structure will allow us to state whether Nb is a metal, semiconductor, or insulator, depending on whether there is a band gap or not. Here, the dispersion and convergence of bands at the Fermi level signify that Nb is a metal since free electrons are available for conduction.

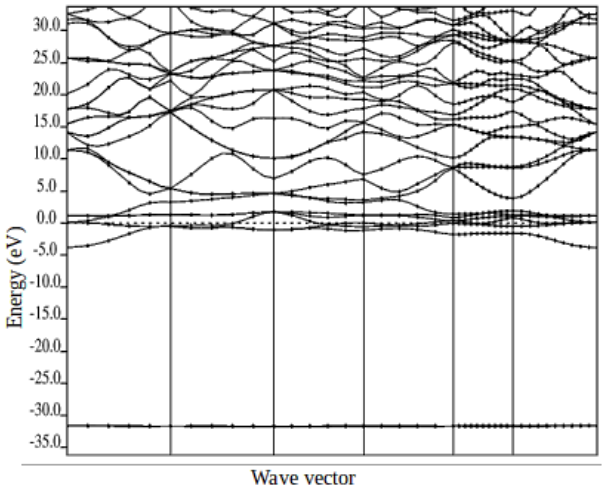

Fig. 3. Band Gap of Nb.

2.5. Partial Density of States

The Partial Density of States (PDOS) extends the DOS concept by assigning specific electronic states to individual atomic orbitals or elements within the crystal. From the PDOS, one can extract information about the contribution of different atoms or orbitals to the total electronic structure and recognize bonding and antibonding states. Figure 4 shows the participation of different Nb orbitals, 1s, 2s, 3p, and 4d, in electronic states. The 4d states of Nb contribute significantly near the Fermi level, indicating that Nb's conduction properties are mainly influenced by its d-electrons. This is characteristic of transition metals. Peaks occurring before the Fermi energy are associated with bound states, which do not contribute to conduction directly but still play an important role in bonding and structural integrity. The states beyond the Fermi level represent unoccupied orbitals, thus showing the possible energy levels electrons can take after excitation.

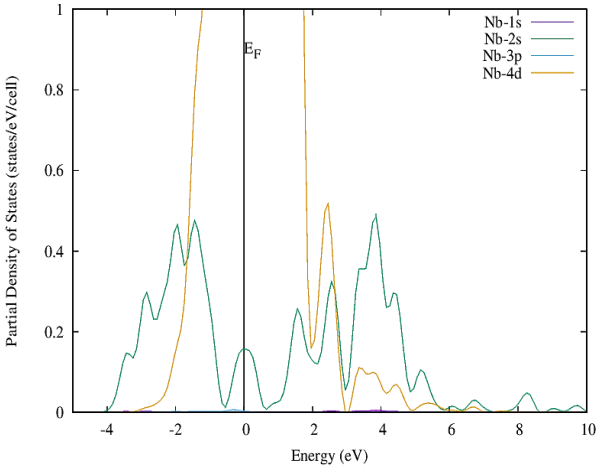

Fig. 4. Partial Density of States of Nb.

Conclusion

The DFT approach applied reveal the mechanical, phonon dispersion, and electronic properties of Nb in this research. Such a multiple approach gave a detailed atomic-level insight into the behaviour of Nb with the necessary insights for basic scientific interests and advanced technological applications. For Mechanical Properties, our simulations showed that the metal Nb was very stable regarding mechanical strength, as the selected elastic constants revealed. These values manifest the potential ability to withstand high stresses, hence recommend Nb for practical applications in such stress-prone environments. The calculated bulk modulus, shear modulus, and Young's modulus are all in good agreement with available experimental data, which proves the reliability of our computational approach. The mechanical robustness associated with a high modulus of Nb renders it useful in aerospace, automotive, and industrial machinery, where failure of materials is unsupportable.

For Phonon Dispersion, our analysis leads to necessary conclusions about the dynamic stability of the examined Nb. The absence of imaginary frequencies across the whole phonon dispersion implies that Nb is dynamically stable. This fact is very important since it assures that Nb will maintain its structure against these high thermally induced factors, which is very crucial for applications under high-temperature conditions. The calculated phonon DOS also assisted in understanding the thermal properties, particularly the specific heat capacity and thermal conductivity, which are required for thermal management in electronic devices and high-temperature industrial processes.

For the Electronic properties, the metallic character of Nb could be further evaluated through its band structure and DOS. It indicates that Nb can support a high density of free electrons because the density of states at the Fermi level is quite significant, and hence it should be a good electrical conductor. This suggests that, in Nb, the d orbitals make a significant contribution to the electronic state near the Fermi level, which is of interest in the investigation of electronic properties. This information is very significant for superconducting applications, where Nb is an incontestable material. In this light, the current study provides an exemplary insight into the electronic interactions making Nb suitable for superconducting applications. The information revealed in this study will be important for the development of new types of Nb alloys and composites that can find tailored properties suitable for specific industrial uses.

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Теоретичне моделювання механічних властивостей, фононної дисперсії та пов'язаних електронних кристалічних властивостей ніобію: DFT-дослідження

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У роботі досліджено механічні властивості, фононну дисперсію та електронні властивості ніобію (Nb) з використанням теорії функціонала густини (DFT). За допомогою програмного пакета Quantum ESPRESSO виконано комплексні DFT-розрахунки для прогнозування властивостей Nb на атомному рівні. Механічні характеристики оцінювали шляхом обчислення пружних сталих, об'ємного модуля, модуля зсуву та модуля Юнга. Фононні спектри було отримано з використанням теорії збурень у межах DFT (DFPT) для оцінки динамічної стабільності. Електронні властивості проаналізовано за допомогою зонної структури та густини електронних станів (DOS). Отримані результати свідчать, що ніобій характеризується високою механічною стабільністю, а пружні сталі підтверджують його стійкість до значних механічних навантажень. Аналіз фононної дисперсії виявив наявність уявних частот, що підтверджує динамічну нестабільність структури. Дослідження електронної структури показало металеву природу Nb із суттєвим внеском d-орбіталей поблизу рівня Фермі, що зумовлює його високу електропровідність. Загалом результати роботи поглиблюють розуміння властивостей ніобію та надають важливі атомарні уявлення, необхідні для подальших експериментальних досліджень і розробки матеріалів для передових технологічних застосувань.

Ключові слова: ніобій, DFT, механічні властивості, фононна дисперсія, густина електронних станів (DOS).