Study of structural, mechanical and electronic properties of the 2H-$NbSe_2$ alloy using density functional theory approach

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1. Introduction

The layered transition metal dichalcogenide 2H-$NbSe_2$ is of considerable interest due to its metallic conductivity, superconducting properties, and potential applications in nanoelectronics [1, 2]. Understanding the relationship between its mechanical and electronic properties is essential for strain-engineered functional materials.

2. Methodology

In this work, the structural, mechanical, and electronic properties of 2H-NbSe2 were investigated using density functional theory (DFT) as implemented in the Quantum Espresso package. The exchange–correlation effects were treated within the generalized gradient approximation (GGA). A plane-wave basis set and periodic boundary conditions were employed.

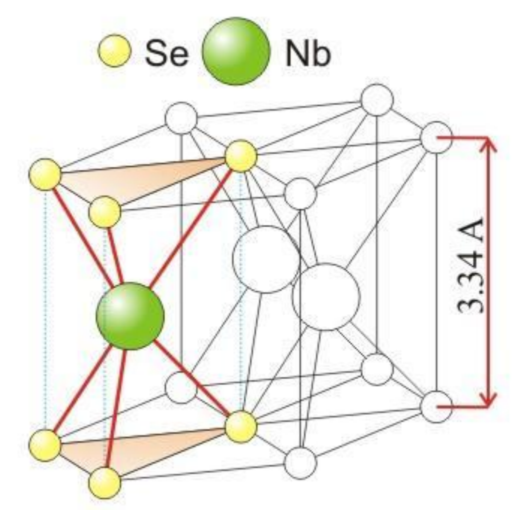

Fig. 1. Crystal structure of the 2H-$NbSe_2$

3. Results and discussion

The optimized lattice parameter was found to be a = 3.445 Å, which is in good agreement with available experimental data [1]. The calculated elastic constants (C_{11}, C_{12}, C_{13}, C_{33}, C_{44}) satisfy the mechanical stability criteria for hexagonal crystals. The derived bulk, shear, and Young's moduli indicate moderate stiffness of the material. The Pugh ratio B/G = 1.18 suggests a brittle mechanical behavior under ambient conditions, consistent with the layered nature of the compound.

Compound	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}
2H-$NbSe_2$	150	42	18	55	5,5

Table. 1. Calculated Elastic Constants (C_{11}, C_{12}, C_{13}, C_{33} and C_{44}) in Gpa for 2H-$NbSe_2$

The effect of small symmetric displacements of Se atoms (±1%) was analyzed. These deformations lead to noticeable changes in the shear modulus and longitudinal stiffness, indicating a pronounced sensitivity of the mechanical response to local atomic distortions.
Electronic structure calculations confirm the metallic nature of 2H-$NbSe_2$. The density of states near the Fermi level is dominated by Nb d–states. Variations in the interlayer spacing affect the width and position of the Nb d–band near the Fermi level, demonstrating a coupling between mechanical deformation and electronic properties.
The obtained results highlight the interplay between structure, mechanical response, and electronic behavior in 2H-$NbSe_2$. This coupling suggests the possibility of tuning electronic properties by controlled strain, which is of interest for nanoelectronic and strain-engineered applications. The results are consistent with previously reported theoretical and experimental studies of layered transition metal dichalcogenides [1–4].

References:

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