

Calculations of Electronic Structural and Elastic Properties of VX_3 ($X = \text{Pt, Pd, Rh, Ir, Os}$) Compounds Using First Principles Study

Khaled Cheikh¹, Wahiba Metiri²,

¹*Département de Génie mécanique, Faculté de Technologie, Université 20 août 1955-Skikda BP 26, Route El-Hadaiek, 21000 Skikda, Algeria*

²*Département de Physique, Faculté des Sciences, Université 20 août 1955-Skikda BP 26, Route El-Hadaiek, 21000 Skikda, Algeria*

Email 1 - kh.cheikh@univ-skikda.dz

Email 2 - w.metiri@univ-skikda.dz

Introduction :

Transition metal trihalides with the general formula VX_3 (where $X = \text{Pt, Pd, Rh, Ir, Os}$) represent an important class of materials with potential applications in catalysis, electronics, and magnetic devices due to their diverse physical properties. These compounds crystallize in layered structures that can exhibit unique electronic and mechanical behavior. Understanding their electronic structure and elastic properties is essential for exploring their suitability in technological applications. In this work, we employ density functional theory (DFT) calculations using the WIEN2k code to systematically study the electronic and elastic properties of VX_3 ($X = \text{Pt, Pd, Rh, Ir, Os}$). Exchange-correlation effects were treated using the Generalized Gradient Approximation (GGA) in the Perdew-Burke-Ernzerhof (PBE) scheme. Muffin-tin radii (R_{MT}) were carefully chosen to avoid overlap, and the plane-wave cutoff parameter $R_{\text{MT}} \cdot K_{\text{max}}$ was set to 7.0. A dense k-point mesh of $12 \times 12 \times 12$ was used to sample the Brillouin zone for accurate electronic and elastic property determination.

Results and discussion:

Structural Optimization:

The optimized lattice constants for each VX_3 compound are in good agreement with available experimental data or previous theoretical reports. A general trend of decreasing lattice parameter is observed with heavier transition metals, consistent with stronger bonding and smaller atomic radii across the series from Pd to Os.

Electronic Properties:

The electronic band structure and total density of states (DOS) for each compound reveal metallic or semiconducting character depending on the transition metal. VX_3 compounds with Pd and Rh

show a narrow band gap or semimetallic behavior, while those with Pt, Ir, and Os are clearly metallic with significant density of states at the Fermi level. In all cases, the valence band is predominantly formed by V 3d and X d orbitals, indicating strong hybridization. The degree of metallicity increases with the heavier elements (Ir, Os), suggesting enhanced electrical conductivity and potential for catalytic activity.

Elastic Properties:

The elastic constants C_{11} , C_{12} , and C_{44} were computed for all compounds to evaluate mechanical stability. All VX_3 compounds satisfy the Born criteria for mechanical stability in cubic systems ($C_{11} > 0$, $C_{11} > |C_{12}|$, $C_{44} > 0$). The calculated bulk modulus (B), shear modulus (G), and Young's modulus (E) indicate that PtX_3 and OsX_3 are the stiffest among the series, with higher resistance to volume and shape changes. The B/G ratio further reveals ductile behavior for PtX_3 and IrX_3 , whereas VX_3 compounds with Pd and Rh lean toward brittleness.

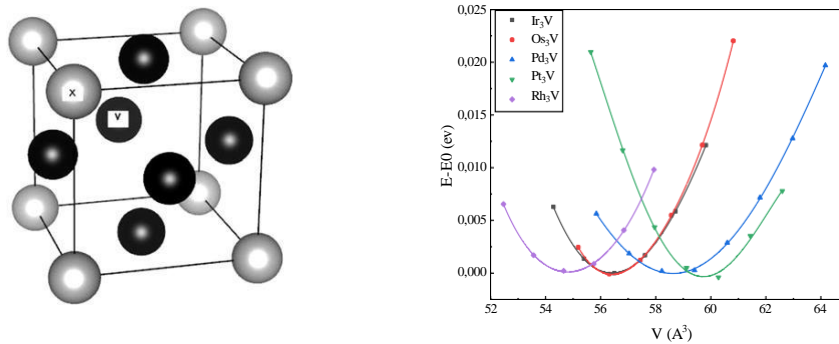


Fig. 1. (a)Crystal structure and **(b)** Energy vs volume variations of X_3V (X=Pt, Pt Rh Ir Os) alloys.

Conclusion :

This DFT-based study provides a detailed analysis of the structural, electronic, and mechanical properties of VX_3 (X = Pt, Pd, Rh, Ir, Os) compounds. The results show that electronic and elastic properties can be tuned effectively by selecting appropriate transition metals. Pt and Os variants show superior metallic behavior and mechanical hardness, whereas Pd and Rh versions exhibit semiconducting tendencies and lower stiffness. These findings offer useful insights into the design of transition metal-based materials for electronic and structural applications.

Références :

- [1] N. Arlkan, A. yigör, A. Candan, M. Özduran, A. Karakoç A. Bouhemadou, S. Bin-Omran, and N. Guechi “Met. Mater. Int., Vol. 20, No. 4 (2014), pp. 765~773doi: 10.1007/s12540-014-4022-1
- [2] K. Chen , L.R. Zhao , J.S. Tse , J.R. Rodgers Physics Letters A 331 (2004) 400–403
- [3] TF Wang, C Ping, YH Deng and BY Tang Transactions of Nonferrous Metals Society of China Volume 21, Issue 2, February 2011, Pages 388-394
- [4] Chen, L. R. Zhao, and John S. TseJournal of Applied Physics 93, 2414 (2003) doi: 10.1063/1.1540742