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First-principles study of structural stabilities, elastic and electronic properties of transition metal monocarbides (TMCs) and mononitrides (TMNs)

Abstract

The structural stabilities, elastic and electronic properties of 5d transition metal mononitrides (TMNs) XN with (X = Ir, Os, Re, W and Ta) and 5d transition metal monocarbides (TMCs) XC with (X = Ir, Os, Re and Ta) were investigated using the full-potential linear muffin-tin orbital (FP-LMTO) method, in the framework of the density functional theory (DFT) within the local density approximation (LDA) for the exchange correlation functional. The ground state quantities such as the lattice parameter, bulks modulus and its pressure derivatives for the six considered crystal structures, Rock-salt (B1), CsCl (B2), zinc-blend (B3), Wurtzite (B4), NiAs (B81) and the tungsten carbides (Bh) are calculated. The elastic constants of TMNs and TMCs compounds in its different stable phases are determined by using the total energy variation with strain technique. The elastic modulus for polycrystalline materials, shear modulus (G), Young's modulus (E), and Poisson's ratio (ν) are calculated. The Debye temperature (θD) and sound velocities (vm) were also derived from the obtained elastic modulus. The analysis of the hardness of the herein studied compounds classifies OsN - (B4 et B81), ReN - (B81), WN - (B81) and OsC - (B81) as superhard materials. Our results for the band structure and densities of states (DOS), show that TMNs and TMCs compounds in theirs energetically and mechanically stable phase has metallic characteristic with strong covalent nature Metal-Nonmetal elements.

Keywords — A. Carbides, A. Nitrides, C. Ab initio calculations, C. Hardness, D. Band-structure, D. Elastic properties