Abstract Submitted
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Structural, mechanical and electronic properties of 3d transition metal nitrides in cubic zincblende, rocksalt and cesium chloride structures: a first-principles investigation[1] SANJAY KHARE, ZHI LIU, University of Toledo, XIUQUAN ZHOU, University of Maryland, DANIEL GALL, Rensselaer Polytechnic Institute — We report systematic results from ab initio calculations on three cubic structures, zincblende (zb), rocksalt (rs) and cesium chloride (cc) of the ten 3d transition metal nitrides. We computed lattice constants, elastic constants, their mechanical moduli and ratios, which are in good agreement with experiments. All nitrides, except for zb-CrN, rs-MnN, rs-FeN, cc-ScN, cc-NiN and cc-ZnN, were found to be mechanically stable. A clear correlation in the atomic density with the bulk modulus (B) was observed with maximum values of B for FeN in zb, MnN in rs, and CrN in cc. The shear modulus, Young's modulus, H_V and indicators of brittleness showed similar trends and all showed maxima for cc-VN. The calculated value of H_V for cc-VN was about 30 GPa, while the next highest values were for rs-ScN and rs-TiN, above 24 GPa. A tendency for anti-correlation of the elastic constant C_{44}, which strongly influences stability and hardness, with the number of electronic states around the Fermi energy, was observed. This work has been published as Liu et al., J. Phys.-Condens. Matter 26, 025404 (2014).

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Zhi Liu
University of Toledo

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