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Puzzle of c-WN phase stabilization

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Abstract : In this paper, we present first-principles calculations that compare structural and electronic properties of WN in the NaCl and NbO phases. Our results predict that the NbOstructure of WN is more stable than the NaCl structure without defects, where the enthalpy of formation per formula unit Hf =-0.872eV and 0.616eV for NbO and NaCl structures, respectively. Moreover, the calculated lattice parameters of c-WN are a= $4.35A^\circ$ and a= $4.11A^\circ$ for NaCl and NbO phases, respectively. It is very clear that the lattice parameter obtained for c-WN in NbO is invery good concordance with that reported experimentally of a = $4.14A^\circ$. Although the formation energy calculations support the hypothesis of the stability of the NbO phase, the experimental xrayphotoelectron spectroscopy (XPS) electron density of states for valence band spectra corresponds to that density of states calculated for c-WN in NaCl phase. Based on this comparison, more consideration must be taken into account to elucidate this superimental spectra.

Keywords : Cubic Tungsten nitride ceramics, Firstprinciples calculations, Formation energy