Puzzle of c-WN phase stabilization

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Abstract : In this paper, we present first-principles calculationsthat compare structural and electronic properties of WN inthe NaCl and NbO phases. Our results predict that the NbOstructure of WN is more stable than the NaCl structure withoutdefects, 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°and a=4.11A° for NaCl and NbO phases, respectively. It is veryclear that the lattice parameter obtained for c-WN in NbO is invery good concordance with that reported experimentally of a =4.14A° . Although the formation energy calculations support thehypothesis of the stability of the NbO phase, the experimental xrayphotoelectron spectroscopy (XPS) electron density of statesfor valence band spectra corresponds to that density of statescalculated for c-WN in NaCl phase. Based on this comparison,more consideration must be taken into account to elucidate thisissue.

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