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Mechanical Properties of Ternary Metal Nitride Ti1-xTaxN Alloys from First-Principles

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Abstract : We investigate by first-principles pseudo-potential calculations the composition dependence of lattice parameter, hardness and elastic properties of ternary disordered solid solutions Ti(1-x)Ta(x)N (1>=x>=0) with B1-rocksalt structure. Calculations use the coherent potential approximation with the exact muffin-tin orbitals (EMTO) and hardness formula for multicomponent covalent solid solution proposed. Bulk modulus B shows a nearly linear behaviour whereas not C44 and C′=(C11-C12)/2 that are not monotonous. Influences of vacancies on hardness of off-stoichiometric transition-metal nitrides TiN(1−x) and TaN(1−x) are also considered.

Keywords : transition metal nitride materials, elastic constants, hardness, EMTO
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