Theoretical prediction of the electronic and thermodynamic properties of YN-ZrN solid solutions

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Abstract

In this study, the results of structural parameters, electronic structure, and thermodynamic properties of the $Zr_xY_{1-x}N$ solid solutions are presented. The effect of zirconium composition on lattice constant, and bulk modulus shows nonlinear dependence on concentration. Deviations of the lattice constant from Vegard's law and deviations of the bulk modulus from linear concentration dependence were found. Our findings indicate that the $Zr_xY_{1-x}N$ solid solutions are metallic for x = 0.25, 0.5, 0.75. The calculated excess mixing enthalpy is positive over the entire zirconium composition range. The positive mixing enthalpies for $Zr_xY_{1-x}N$ alloys indicate the existence of miscibility gaps and spinodal decompositions. The effect of temperature on the volume, bulk modulus, Debye temperature, and the heat capacity for $Zr_xY_{1-x}N$ alloys were analyzed using the quasi-harmonic Debye model. Results show that the heat capacity is slightly sensitive to composition as temperature increases.

Keywords

density functional calculations, electronic properties, solid solutions, structural properties, thermodynamic properties