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Structural and thermodynamic properties of Zr-Nb-Co

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More advanced Zr-based alloys are being developed for the more severe operating conditions such as higher burn-up and increased operation temperature, this is due to their good resistance to corrosion and high melting point. In this work, density functional theory have been used to investigate the structural and thermodynamic properties of Zr-Nb-Co system at various concentrations. We used the virtual crystal approximation to introduce small Co content on different Zr-Nb composition, Zr₇₈Nb₂₂, Zr₉₇Nb₃, Zr_{98.1}Nb₂, Zr₉₉Nb₁, We found that the increase in Co concentration enhances the stability of the compound with the Zr₇₈Nb₂₂ being the most preferred composition, and the alloy is stable only at a small Co concentration of about 3%. The structure were also confirmed using XRD patterns. we also found that the Zr₇₈Nb<sub>17<sub>Co₃ structure is stable above 900K

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