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Thermodynamic and mechanical stability studies of Zr-Nb(Co) alloys

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Abstract content
   (Max 300 words)
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Knowledge of phase diagram and thermodynamic properties is important in many applications. We present the Zr₇₈Nb_{22-x}Co_x alloys, using the virtual crystal approximation as embedded in the Density Functional Theory (DFT), employing the Perdew Burke and Enzerhof (PBE) pseudopotentials. Their equilibrium lattice parameters, heats of formation, elastic properties and the density of states were evaluated to check the relative stability of competing phases. The smaller amount of Co is favourable for doping ZrNb alloy since it favours cladding purposes and is good for avoiding hydride attack. Furthermore, alloying with cobalt is significant since it is recommended for preparation of magnetic, wear-resistant and high strength alloys. The idea is to develop suitable materials which can withstand aggressive environments and high temperature operations.

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