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Preference of Co and Sn additions on Zr- x Nb alloy

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Zr-based alloys are aimed 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. Most of these Zr alloys contains Nb as the major alloying element, which is recommended for developing new fuel cladding materials since it is an effective strengthening element. This study uses *ab initio* method to investigate the effect of Co and Sn addition on Zr-Nb alloy, their thermodynamic and mechanical properties were calculated to understand the effect of alloying. In the quest to enhance the resistance to corrosion of the advanced future cladding nuclear material, we have investigated the Zr-N x b alloys which allow to introduce small Co and Sn contents at less computational costs. The Zr-N x b alloys with a higher percentage of Nb ($x \gg 5$) causes the deterioration of corrosion properties. We have noted significance of alloying Zr-N x b at small concentrations. It was found that the Co and Sn addition on the Zr-N x b alloy at small concentrations are more preferred for thermodynamic and mechanical stability of the alloy system. Their elastic stability was also evaluated at high temperature and revealed that the Sn addition is more preferred and may be applicable in the development of future cladding nuclear materials.

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