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Computational modelling of Zr-Nb alloys by solid solution approach

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<p>We use density functional theory to investigate the structural, elastic properties and energetic stabilities of Zr, Nb and its alloys in the alpha and beta phases, employing pseudopotential plane wave methods within the Pardew-Burke-Ernzerhof Generalized Gradient Approximation (PBE-GGA). The structures were fully optimized in a non-magnetic state, allowing atomic positions, cell volume and shape to change. Lattice parameters for the pure phases gave excellent agreement with the available experimental data. We also found that the phonon dispersions curves display soft-modes for the metastable beta-Zr phase which is lacking on the alpha-Zr and beta-Nb, condition of mechanical stability. The solid solution calculations show that an increase in the Nb contents destabilizes the structures in both the alpha and beta phases. Interestingly, the calculated elastic moduli for Zr-2.3

Level (Hons, MSc,
   PhD, other)?

Hons

Consider for a student
   award (Yes / No)?

Yes

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

Yes

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