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First-principles study on the effect of Pt addition on the stability of B2 Ti50Ru50 – a supercell approach

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Abstract: The discovery of new advanced structural materials to meet the aggressive evolving engineering structural demands can be achieved through the integration of computational thermodynamics and validated experimental activities to optimize the existing materials. Nitinol, Ti50Ni50, is a commercial shape memory alloy (SMA) widely used in structural applications is known to possess shape memory effect and excellent super-plasticity. Materials that display such unique structural properties are usually referred to as SMAs, with a tendency of recalling their prior crystal structure and properties if subjected to a conducive environment such as temperature. Though Nitinol is widely known as an alloy with shape memory effect (SME), it has drawn back such as being limited to low-temperature structural applications. So any advanced structural materials that could overcome Nitinol's structural application's limitation stand a good chance to be considered as high-temperature shape memory alloys (HTSMAs). This SME is driven by a diffusionless phase transition, from an ordered high-temperature B2 phase to disordered low-temperature martensite phases (L10/B19/B19'), present in CsCl compounds. Whilst Ti50Ru50 also consist of B2 at high-temperature, it remains ordered with no phase transition to 0 K. Owing to platinum's nobility and excellent malleability, this work employed a supercell (SC) approach to pin-track B2-Ti50Ru50-xPtx ternary compositions with the prospect to stimulate SME on stable B2-Ti50Ru50 by substituting some of Ru atoms with Pt atoms. In pursuit of such advanced structural materials with SME, we evaluated the thermodynamic, mechanical, electronic and lattice dynamic stability using first-principles calculations.

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YES

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MSc

Primary authors: Mr NGOBE, Bongani (WITS and MINTEK); Dr PHASHA, Maje (MINTEK); Dr MOLEPO, Mahlaga (University of the Witwatersrand)

Presenter: Mr NGOBE, Bongani (WITS and MINTEK)

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