



Contribution ID: 124

Type: Oral Presentation

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

Wednesday, 5 July 2023 11:20 (20 minutes)

Keywords: Advanced structural materials, First-principles calculations, Density functional theory (DFT), Phase stability and Phase transition

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-xPt_x 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.

Apply to be considered for a student ; award (Yes / No)?

YES

Level for award;(Hons, MSc, PhD, N/A)?

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)

Session Classification: Theoretical and Computational Physics

Track Classification: Track G - Theoretical and Computational Physics