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The Ab Initio Study of Ti50Pt50-xHfx (x = 6.25, 18.75, 25) Potential Shape Memory Alloys

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The ab initio density functional theory approach was employed to study the effect of Hf addition to the TiPt binary shape memory alloys (SMAs). SMAs have the ability to retain its original shapes after deformation and have been widely used in the fields of engineering and medicine due to their shape memory effect (SME) and super-plasticity which are displayed in martensitic transformations. Previously, the B2 TiPt system was reported to be unstable with respect to negative C′ and phonon soft modes. In this work, a supercell approach method in VASP was used to substitute Pt with 6.25, 18.75 and 25 at.% Hf in the TiPt. We have found that the calculated heats of formation predicted that 6.25 at.% Hf to be thermodynamically stable structures. The calculated elastic properties confirmed stability of the TiPtHf at different concentration of Hf content with all the Cij being positive. It is thus observed that Hf addition enhances the stability of the B2 TiPt. Moreover, phonon dispersion curves indicated that increasing the Hf content in the system stabilizes the structure with no soft modes observed. These findings suggests that Ti50Pt43.75Hf6.25 has shown potential for alloy development with promising industrial application.

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MSc

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