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The elastic properties and the phonon dispersions of TiPtCo shape memory alloy using the supercell approach

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Abstract :

Shape memory alloys (SMAs) are classified as a group of metallic materials that has the ability to retain or remember their original shape or size when subjected to the appropriate thermal deformation processes. In general, these materials can easily be elastically or plastically deformed at some relatively low temperature, and upon exposure to some higher temperature can return to their original shape. The effect of substituting Pt with Co as the third element in the TiPt shape memory alloy system has been investigated using the supercell approach. The elastic properties of the TiPtCo high temperature SMAs were investigated by using the *ab initio* approach employed in VASP. Furthermore the electronic structure mechanisms behind the elastic properties are discussed based on the phonon dispersions.

Award :

no

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Paper :

yes

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