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The ab initio study of Ti50Pt50-xTax (x = 6.25, 18.75, 25 at.%) shape memory alloys

The first principle density functional theory approach was employed to study the effect of Ta addition on the TiPt shape memory alloys (SMAs). SMAs have the ability to remember their shapes after deformation, and this is due to their shape memory effect and super elasticity properties. They have potential to operate as high temperature shape memory alloys since they possess a reversible martensitic transformation. All the intensive calculations in this study are carried out on the Lengau cluster of the Centre for High Performance Computing (CHPC), whereby we use VASP code embedded in Material design.We employed the plane-wave pseudopotential method within generalized gradient approximation parameterized by Perdew, Burke and Enzerhof using the supercell approach within VASP code. The embedded atomic model based on LAMMPS code was used to determine the temperature effect on the Ti50Pt50-xTax (6.25, 18.75, 25 at.%) structures. The results show that equilibrium lattice parameter increases as the Ta content is increased in the system and the calculated elastic properties are found to be mechanically stable with all the Cij's being positive. The phonon dispersions of the structures are also calculated.

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