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Computational modelling studies of Ti₅₀-Pt_{50-x}-Nb_x alloys

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Abstract content
   (Max 300 words)
Formatting &
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Shape Memory Alloys (SMAs) are materials which have the ability to return to the initial shape when heated beyond certain temperatures. The behaviour is unique due to the superelasticity and shape memory effect which is possessed by the materials. NiTi is one of the materials that have received wide technological applications but it is limited by its low transformation temperature of 100℃. This has called for the growing demand of SMAs which can be used at high temperatures in the transportation, energy, and systems and control industries, TiPt was found to be amongst the potential high temperature shape memory alloys (HTSMAs) which can be used since its transformation temperature is around 1000℃.
In this work Nb was substituted on the Pt sublattice to check its effect on the martensitic transformation temperature. The Ti₅₀-Pt_{50-x}-Nb_x ternaries were determined using the virtual crystal approximation. The investigated structures were optimized and their equilibrium lattice parameters and formation energies were calculated. The lattice parameters were found to be fluctuating minimally with an increase in the Nb concentration. The elastic properties and the density of states for the Ti₅₀-Pt_{50-x}-Nb_x ternaries were also calculated.

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Level for award
 (Hons, MSc,
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Hons

Main supervisor (name and email)
and his / her institution

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