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Mechanical properties and temperature dependence of B19Ti_{50-x}Zr_xPt₅₀ shape memory alloys

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A molecular dynamic study of Ti_{50-x} Zr_x Pt₅₀ as potential high temperature shape memory alloy has been performed using the LAMMPS code. The lattice dynamics, elastic properties and temperature dependence were deduced to determine the effect of ternary addition with Zr on the Ti sub-lattice at varied temperature range. It was found that the lattice parameter increases with Zr addition, the thermodynamic stability was observed at 5 at. % Zr. Furthermore, the elastic properties showed positive shear modulus for concentrations range 5 - 25 at. % Zr, indicating stability of the structures and instability above 25 at. % Zr concentrations. More importantly, we observed a martensitic transformation behaviour for Ti_{50-x} Zr<sub>Xc<sub>Pt₅₀ (x= 3.125, 9.375) at around 900K.

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

Yes

Level for award

- (Hons, MSc,

- PhD, N/A)?

PhD

Main supervisor (name and email) < br>and his / her institution

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Would you like to
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Yes

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