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## **Mechanical properties of TiPt-M (M= Zr and Hf) for actuators and turbine applications**

Titanium and its alloys, with their high strength to weight ratio and high-temperature properties, are used extensively by the aerospace industry. They are typically utilized for airplane parts and in medical industries. Recently, demand for shape memory alloys, which can be used at high temperature has increased. The first principle approach was employed to investigate the effect of the third element Zr and Hf on the equiatomic TiPt shape memory alloy. The solid solution approach in CASTEP was evaluated at the CHPC cluster, on Accelrys queue, using 32 cores to substitute Ti with Zr and Hf on a TiPt structure and evaluate their thermo-dynamic and mechanical stabilities. It was found that partial substitution of Zr was the most stable structure as compared to the Hf in terms of heats of formation. The Zr was found to be more ductile than Hf, their C' shear modulus was found positive and completely anisotropic. The coefficient of linear expansion showed that the Hf expanded more over a given temperature range.

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