Contribution ID: **60** Type: **Student Micro-talk**

Understanding the effects of Ni addition on the stability of B2 TiPd system using DFT approach

Abstract

The TiPd alloy is one of the promising candidate for high temperature shape memory applications with the martensitic transformation temperature from B2 to B19 at 823 K. Previous studies showed that the B2 TiPd is unstable since it displays negative C′ which resulted in poor shape memory behaviour. In order to enhance the properties, the effects of partial substitution of Pd with Ni are being investigated. The stability of the Ti50Pd50-xNix structures was determined with respect to their heats of formation, elastic constants and moduli using density functional theory. It was found that the heats of formation increase with an increase in Ni, indicating stability at various compositions. The independent elastic constants revealed that the stability is attained above 43.75 at. % Ni. These results suggest that this dopant reduces the martensitic transformation temperature of the Ti50Pd50 alloy. The calculated moduli confirm that alloying with Ni effectively increases hardness and ductility in the Ti50Pd50 system. These findings can play an important role in future materials in the aerospace industries.

HPC content
Understanding the effects of Ni addition on the stability of B2 TiPd system were achieved by utilizing VASP code in the Medea environment at the CHPC.
The structural, thermodynamic and elastic properties were achieved by utilizing the VASP code.
Application code: VASP
Problem size: 16 atoms
Core count: 48
Computational challenges: calculations are not running most of the time at the CHPC, I am always getting errors.

Student?

Yes

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Session Classification: Micro-talks

Track Classification: Materials Science