Contribution ID: **61** Type: **Oral Presentation**

Investigating the effect of Co addition on the stability of B2 TiPd system using DFT approach

Tuesday, 9 July 2019 10:00 (20 minutes)

The TiPd alloy exhibits thermoelastic martensitic phase transformation above 823 K and has potential for high-temperature shape memory applications. Previous studies showed that this alloy is unstable displaying a negative C′ at room temperature. In order to improve their properties, the effects of partial substitution of Pd with Co are being investigated. The structural, thermodynamic and elastic properties of TiPdCo alloys were simulated using first-principle calculations within the generalized gradient approximation based on density functional theory. The heat of formation increases with an increase in Co concentration, indicating stability at various compositions decrease. The independent elastic constants results revealed that stability is attained at above 31 at. % Co in agreement with the phonon dispersion curves. The calculated moduli confirm that alloying with Co effectively increases hardness and ductility in TiPd systems. These findings can have important implications for future materials design in aerospace industries.

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Session Classification: Physics of Condensed Matter and Materials

Track Classification: Track A - Physics of Condensed Matter and Materials