Rita John et al., J Material Sci Eng 2017, 6:7 (Suppl)
DOI: 10.4172/2169-0022-C1-079

First principle calculations on the effect of addition of X (Co, Rh, Ir) on TiPd

Rita John and **Namitha Anna Koshi**
University of Madras, India

Shape memory alloys are intermetallic compounds that have the ability to recover their original shape upon appropriate thermo-mechanical loading. TiPd, a prominent high temperature shape memory alloy (HTSMA) undergoes martensitic transformation (MT) from the parent B2 (cubic) phase to the product B19 (orthorhombic) phase. We have studied the effect of addition of X (Co, Rh, Ir) on the structural and electronic properties of TiPd shape memory alloys. The site preference of ternary additions X are determined from the calculated formation energy. It was found that X has strong preference for Ti sublattice for the composition considered. The cubic structure of B2 phase is maintained for the substitutional alloying of 6.25% of Ti/Pd sites with X. The density of states (total, site and angular momentum decomposed) are plotted for both $Ti_{43.75}Pd_{50}X_{6.25}$ and $Ti_{50}Pd_{43.75}X_{6.25}$ series. Higher stability of $Ti_{43.75}Pd_{50}X_{6.25}$ is due to the decrease of d states of Ti and X at fermi level with increasing atomic number of X impurities. Though localization effect is more pronounced in $Ti_{50}Pd_{43.75}X_{6.25}$ series with increasing atomic number of X, the number of d states of Ti remains same. It is Ti d states at fermi level that determines the phase stability of these alloys. Also, we have investigated the impact of addition of varying concentration of magnetic impurity Co (6.25, 12.5, 25%) on B2 and B19 phases of TiPd. Band Jahn Teller broadening is observed in $Ti_{25}Pd_{50}Co_{25}$ which is one of the accompanying features of MT. Band structure calculations are consistent with the results of density of states. Hole and electron pockets observed in the band structure are endorsed in fermi surfaces. Charge density contours are plotted which give an idea about electron charge distribution and nature of bonding.

Biography

Rita John is Professor and Head, Department of Theoretical Physics, University of Madras, Chennai, India. She is fulbright Visiting Professor at the Department of Physics and Astronomy, Texas Christian University, Fort Worth, Texas, USA (2014). She has been teaching condensed matter physics for graduate students over 18 years. The book, '*Solid State Physics*' authored by her and published by Tata McGraw Hill publisher (2014) is used globally by graduate students. She guides PhD, MPhil, MSc and MTech projects. She has over 50 international publications. She is the recipient of various awards and prizes for her academic and research contributions.

ritajohn.r@gmail.com

Notes: