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Cooperation between computational modelling and experimental characterization of materials

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Lately, with the high demand of production and commercialization the need to combine both computational modelling techniques and experiments to speed up the process has become a reality. Computational models typically use observation and manipulation in the same ways as physical experiments, because their goals are often the same. The advantages of computational modelling comes with low cost for raw materials, safety and saves time with procedures of synthesis and characterization in the laboratory. The recent work looks into how CHPC has been used in preparing the models and tested using experiments. Ti-based alloys are considered to be the most attractive metallic materials for aerospace and automobile applications. TiPt is one of the promising shape memory alloys that can be used at high temperatures due to its transformation temperature of 1000 0C. However, the binary alloy has been found to be mechanically unstable and exhibit very low shape memory effect attributed to low critical stress for slip deformation compared to the stress required for martensitic transformation. We present some of the results obtained using both computational modelling and experimental approaches on the alloy wherein addition of a third element to the system is investigated.

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