Paths of phase transformations in titanium alloys based on four dimensional structural description

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Phases involved in the solid state transformations of titanium alloys pertain to \(\alpha\) (P6\(5\)3/mmc), \(\beta\) (Im3m), \(\omega\) (P6/mmm), \(\alpha'\) (P6\(3\)/mmc), and \(\alpha''\) (Cmcm) phases [1]. A unified structural description of transformations involving \(\alpha\), \(\beta\), and \(\omega\) phases has been discussed [2]. The model in reference [2] employs higher dimensional crystallographic formalism and utilises a single scalar order parameter \(\eta\). The value of \(\eta\) in the model depends upon an angular distortion \(\theta\) around a three-fold axis. Such a model has been successful in predicting paths of \(\beta\) \(\omega\), \(\alpha\) \(\omega\), and \(\beta\) \(\alpha\) transformations.

The same model has been shown to successfully recover the structural attributes of \(\alpha''\) phase, including identification of the paths of \(\beta\) \(\alpha''\) and \(\alpha'\) \(\alpha''\) transformations. The results for the same shall be presented in this work. It will be shown that structural description of \(\alpha'\) phase requires orthogonal 4D hyperlattice parameters to be \(t_1 = t_2 = t_3 
eq t_4\) while the \(\alpha''\) phase is modelled by \(2t_1 = t_2 
eq t_3 
eq t_4\), for the same value of \(\eta\). This implies a continuous transformation of \(\alpha''\) \(\alpha'\), whereas a structural discontinuity exists in the path of \(\beta\) \(\alpha''\) transformation. This is in agreement with experimental findings reported elsewhere [3]. The findings are also consistent with group-subgroup relationships [4] based on argument of symmetry breaking. A schematic representation of the identifiable paths of transformation in titanium alloys has been depicted in Fig 1. This includes additional path IV not reported in reference [2]. It shall be demonstrated that our model is sufficiently general to describe the entire gamut of structural transformations observed in titanium alloys, including zirconium and hafnium alloys. The general 4D model proposed in this work helps advance our understanding of structural transformations in alloys by providing a unified basis.

Figure 1. Pathways of possible structural transformations in titanium alloys.