Metalss, which form the significant proportion of the engineering materials, are in general, crystalline. Deformation and phase transformation are two principal modes of microstructural control/evolution in these materials. The crystalline nature of these materials makes ‘how these crystals are oriented’ influence the material behavior in the deformation and/or phase transformations. The role of the crystal orientation is even more dominant in case of materials with low symmetry such as Zirconium, a hcp metal. A thorough understanding of the role of orientation in these phenomena can go a long way in optimization of the fabrication processes of the Zr based components used in the nuclear reactors. Present thesis is aimed at furthering the understanding of the phenomena of deformation and phase transformation in these alloys, using a combination of experimental and modeling techniques with a focus on the role played by the local crystal orientation.

For studying the $\beta \rightarrow \alpha$ phase transformation (one of the most prominent phase transformation in Zr alloys), an algorithm for automated reconstruction of parent microstructure, from the microtexture data of product phase, was developed. It uses the microtexture (local crystal orientation) information of the product phase to reconstruct the high temperature phase orientation information and thus its microstructure. It involves identifying triplets of neighboring product grains with a common parent variant and linking such neighboring triplets with a generalized misorientation criterion. The algorithm was successfully applied for quantifying the variant selection during $\beta \rightarrow \alpha$ transformation. The role of variant selection in determining the grain boundary nature of the transformed product was demonstrated.

Another phase transformation of interest in case of Zr is the formation of hydride phase ($\alpha \rightarrow \delta$). Hydride formation in a dual phase microstructure of Zr was studied. Hydrides were found to have preferentially formed along the $\alpha/\beta$ interfaces. Microtexture measurements showed that the orientation relationship between $\alpha$ and $\delta$-hydride phase was $\{0001\}_\alpha \parallel \{111\}_\delta$ and $\langle 2\overline{1}10 \rangle_\alpha \parallel \langle 110 \rangle_\beta$. It was shown that the hydrides have higher preference to form along
such $\alpha/\beta$ interfaces which have one of the low index planes of the $\beta$ phase constituting the interface.

Another mode of microstructural modification i.e., deformation, was studied in terms of role of local orientation on the deformation heterogeneity, role of alloying elements and initial orientation distribution (texture) and microstructure on different modes of deformation (slip and twinning). Orientation and temperature dependent heterogeneous deformation in Zr was investigated for plane strain loading. Extensive degree of strain partitioning was observed between grains of different orientations, particularly in room temperature deformation. Deformation at higher temperatures, however, had shown significant reduction in deformation heterogeneity. Discrete dislocation dynamics simulations, incorporating temperature dependent threshold criterion for the activation of various slip systems, has successfully explained these observations. These simulations have brought out a novel phenomenon whereby dormant slip systems i.e., slip systems on which the applied stress is below critical resolved shear stress, are activated due to interactions with active primary dislocations. It is proposed that this mechanism can play an important role in reducing orientation dependent deformation heterogeneity in hcp materials at high temperatures.

Role of Sn and orientation on the deformation mechanisms of Zr was investigated using in-situ neutron diffraction and complementary electron microscopy techniques. Binary Zr-Sn alloys having fully recrystallized microstructure and typical rolling texture were subjected to in-situ loading and diffraction experiments. Critical stress for the twin nucleation and the extent of twinning were found to be strongly influenced by the Sn content and loading direction (or orientation). Critical plastic strain for the nucleation of twining, however, was observed to be weakly dependent on the Sn content. Results indicate significant plastic slip activity to be a necessary condition for the onset of twinning. Further, the probability of twinning was shown to be a strong function of the initial orientation.

Using Molecular dynamics simulations, dependence of homogeneous nucleation of dislocations on the crystal orientation had been studied. The asymmetry in the critical stress for nucleation of dislocations in tension Vs compression had been brought out. Using a detailed analysis of the defect structures, it had been shown that nucleation of defects on prismatic planes is much more favorable than on the basal or pyramidal planes in case of Zr.