Mechanical Engineering Doctoral Defense

Role of impurities on deformation of HCP crystal: A multi-scale approach

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abstract

Commercially pure (CP) Ti-alloys present excellent corrosion resistance, lightweight, and formability making them attractive materials for expanded use in transportation and medical applications. However, the strength and toughness of CP titanium are affected by relatively small variations in their impurity/solute content (IC), e.g., O, Al, and V. This increase in strength is due to the fact that the solute either increases the critical stress required for the prismatic slip systems ($\{10\bar{1}0\}\langle 1\bar{2}10\rangle$) or activates another slip system ($\{0001\}\langle 11\bar{2}0\rangle, \{10\bar{1}1\}\langle 11\bar{2}0\rangle$). In particular solute additions, such as O, can effectively strengthen the alloy but with an attendant loss in ductility by changing the behavior from wavy (cross slip) to planar nature. In order to understand the underlying behavior of strengthening by solutes, it is important to understand the atomic scale mechanism. This dissertation aims to address this knowledge gap through a synergistic combination of density functional theory (DFT) and molecular dynamics. Further, due to the long-range strain fields of the dislocations and the periodicity of the DFT simulation cells, it is difficult to apply ab initio simulations to study the dislocation core structure. To alleviate this issue we developed a multiscale quantum mechanics/molecular mechanics approach (QM/MM) to study the dislocation core. We use the developed QM/MM method to study the pipe diffusion along a prismatic edge dislocation core. Complementary to the atomistic simulations, the Semi-discrete Variational Peierls-Nabarro model (SVPN) was also used to analyze the dislocation core structure and mobility. The chemical interaction between the solute/impurity and the dislocation core is captured by the so-called generalized stacking fault energy (GSFE) surface which was determined from DFT-VASP calculations. By taking the chemical interaction into consideration the SVPN model can predict the dislocation core structure and mobility in the presence and absence of the solute/impurity and thus reveal the effect of impurity/solute on the softening/hardening behavior in α-Ti. Finally, to study the interaction of the dislocation core with other planar defects such as grain boundaries (GB), we develop an automated method to theoretically generate GBs in HCP type materials.

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