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Effect of Chemistry on Dislocation Core Properties in α-Fe: AN *ab initio*-Based Approach ZHENGZHENG CHEN, NICHOLAS KIOUSSIS, Dept. of Physics, California State Univ., Northridge, NASR GHONIEM, Dept. Mechanical and Aerospace Engr., UCLA, TADASHI HASEBE, Dept. of Mechanical Engr., Kobe Univ., Japan — Screw dislocations in α-Fe and its alloys play an important role on the low-temperature mechanical properties. The solute atom can cause a significant local reconstruction of the dislocation core and therefore affect the mobility. Since direct investigations of the solute-dislocation interaction by first principles calculation remains a difficult problem, we employ a hybrid coupling approach that includes atomistic dislocation modeling with ab initio parameterization of the inter-row interactions, proposed by Suzuki. Using this approach, we have investigated the change of core structure and the $a/2\langle 111\rangle$ screw dislocation mobility induced by impurities of Cu and Cr. We find that Cu induces a change from a non-degenerate (P=0, where P is the core polarization) core structure in α-Fe to a degenerate (P=1) one, while Cr impurity does not change the P at any concentration. We have also studied the behavior of these systems under stress, and found that Cr impurities lower the mobility of the screw dislocation, while Cu induces that the dislocation of Fe-Cu system under stress exhibits a peculiar *stable* $\rightarrow$ *metastable* $\rightarrow$ *stable* transition, and strengthens α-Fe. The above conclusions are supported by molecular dynamics calculation, which also show that Cu impurities, in addition to changing the core polarization, dramatically increase the edge components of screw dislocation in Fe.

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