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Ab-initio Concurrent Multiscale Method to Address Defects in Metals GEORG SCHUSTERITSCH, Harvard University, THOMAS KÜHNE, Johannes Gutenberg University of Mainz, EFTHIMIOS KAXIRAS, Harvard University — We present a concurrent multiscale method for metallic systems based on coupling a region calculated using Kohn-Sham Density-Functional-Theory (KS-DFT) to a macroscopic region employing the Embedded Atom Method (EAM). By construction, our method is particularly well suited for treating defects such as grain boundaries (GBs), dislocations and chemical impurities, where quantum mechanical interactions in a small region near the defect may affect the mechanical properties at the macroscopic scale. Results for two metals, Nickel and Copper, are presented in the context of chemical embrittlement. We study the effects of impurities near GBs and investigate the surrounding strain field. This gives us insights into the role defects play in the underlying physical mechanism of chemical embrittlement.

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