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An *ab-initio* multiscale method to investigate chemical embrittlement of metals GEORG SCHUSTERITSCH, Harvard University, THOMAS KÜHNE, Johannes Gutenberg University of Mainz, EFTHIMIOS KAXIRAS, Harvard University — We present a multiscale method, coupling a small region treated by first-principles quantum mechanics, to a large classical atomistics region. Our method is based on total energy arguments that are applicable to metals. We employ Kohn-Sham (KS) Density Functional Theory (DFT) in the region of interest and couple this to the classical Embedded Atom Method (EAM). Results for the chemical embrittlement of metals due to segregated impurities at grain boundaries (GB) are presented. We study the average interplanar strain surrounding the GB and use this as a measure of the atomic relaxation. We apply our method to study the chemical embrittlement of Cu by Bi and Pb impurities and compare this to the effect of Ag impurities, which are known to segregate to the GB but not embrittle Cu. We find that Bi and Pb weaken and hence embrittle the Cu GB. In contrast Ag impurities at the GB plane increase cohesion.

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