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Interface mobility from interface random walk[1] ZACHARY TRAUTT, MONEESH UPMANYU, Colorado School of Mines, ALAIN KARMA, Northeastern University — Computational studies aimed at extracting interface mobilities require driving forces orders of magnitude higher than those occurring experimentally. We present a computational methodology that extracts the absolute interface mobility in the zero driving force limit by monitoring the one-dimensional random walk of the mean interface position along the interface normal. The method exploits a fluctuation-dissipation relation similar to the Stokes-Einstein relation, which relates the diffusion coefficient of this Brownian-like random walk to the interface mobility. Atomic-scale simulations of grain boundaries in model crystalline systems validate the theoretical predictions, and also highlight the profound effect of impurities. The generality of this technique combined with its inherent spatial-temporal efficiency should allow computational studies to effectively complement experiments in understanding interface kinetics in diverse material systems.

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