A walk along an interface yields its mobility

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In the October 27th issue of *Science*, researchers at Colorado School of Mines and Northeastern University report a novel computational methodology aimed at quantifying the kinetics of interfaces in diverse material systems. The paper, titled "Interface Mobility from Interface Random Walk", addresses computational issues in extracting interface kinetic parameters under experimentally relevant conditions.

Interfaces are an important class of defects whose distribution affects the properties of the otherwise pristine material, both in nature and in technology. This is especially the case in polycrystals, thin films, multiphase materials, and composites, where the mechanical, chemical, and transport properties are sensitive to the underlying interfacial microstructure.

"In fact, tailoring this microstructure is an emerging paradigm for engineering high performance, multifunctional materials," said Zachary Trautt, a graduate student at Colorado School of Mines and the first author in the study.

The interfacial microstructure is subject to several driving forces during material synthesis and function. More often than not, these driving forces are large enough to cause the interfaces to move and the microstructure (or its precursor) evolves. Naturally, controlling the final microstructure requires accurate models that relate the interface motion to the driving forces in effect.

A quantitative measure of interface kinetics is the interface mobility, the

ratio of the interface velocity to the driving force. Past studies on individual homophase crystalline interfaces (or grain boundaries) in several high-purity metals show an interesting trend; the experimental mobilities are orders of magnitude smaller than those extracted via computations. The discrepancy is often attributed to the presence of impurities, fueling speculation that even minute quantities of impurities significantly retard interface motion.

"An often overlooked fact is that computations are limited to tens of nanoseconds," saidMoneesh Upmanyu, co-author and the lead researcher in the study. "As a result, they are performed at driving forces orders of magnitude greater than those commonly observed in experiments," he explained. "This further weakens the comparison, and there is a need to extend the computational studies to more realistic driving forces, and include the effect of impurities."

"Our computational methodology offers a way to address both these challenges, efficiently and with setups that are relatively simple," said Trautt.

The basis for the methodology is the pioneering theoretical work by Einstein, Smulochowski and Langevin on Brownian motion in the early 1900s.

"Just as their study related the dance of macroscopic particles to their diffusivity, the microscopic thermal fluctuations result in interface forces that conspire towards a one-dimensional dance of the average interface position, which in turn yields its mobility in the zero driving force limit," said Alain Karma, also a co-author in the study.

"The technique is remarkably efficient," noted Upmanyu. "The computations on pure aluminum yielded mobilities within a nanosecond, a significant savings in computational resources."

Comparisons with previous experiments and computations reveal that the retarding effect of impurities is much more severe than previously thought. The authors are now working on extending the theory and the computations to directly quantify the impurity drag effect.

The paper is currently available online at: www.sciencemag.org/cgi/content … bstract/314/5799/632 .

Source: Northeastern University