Revealing Line Defect Structures in Crystalline Interfaces

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ABSTRACT

Interfaces, such as phase, grain, and subgrain boundaries, are ubiquitous features of crystalline solids and strongly influence material properties. These interfaces are, invariably, decorated by line defects—both dislocations and disconnections—which, in turn, influence the stability and mobility of the interfaces. However, our ability to predict what line defects are present at interfaces and how interactions among these line defects affect interfacial properties is lacking. In this talk, we discuss two recent advances in theory and modeling of line defects at interfaces which enable new insights. First, we present a new methodology for enumerating all possible line defect structures at semi-coherent interfaces based on the Frank-Bilby equation. Using this methodology, a "menu" of the most favorable structures can obtained and utilized for further analysis. And secondly, we present a new technique called interfacial line defect analysis (ILDA) which automatically identifies and extracts interfacial line defects in atomistic datasets. Using this technique, interfacial line defect structures can be fully analyzed without any user input on the nature of the interface, providing a major capability advancement for the atomistic modeling community.

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