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General model for energy and morphology of crystal interfaces

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ABSTRACT

Understanding interfacial energy between crystal lattices is of great interest in modeling mechanical behavior of multiphase materials and in understanding and predicting interface stability in the context of multimaterial laminate composite design. However, due to the exceedingly complex nature of most interfaces, it is difficult to analyze interfaces in the general case. A semianalyical model is proposed here which attempts to approximate interface energy for the general case and to find the locations of sharp local minima in the energy landscape (”energy cusps”) exactly. It is hypothesized that the coherence (i.e., matched crystal periodicity) across an interface is the dominant effect in interfacial energy. Based on this assumption, an interface energy model is formulated. It is then tested with symmetric tilt boundaries in FCC and BCC materials, as well as for bicrystal orientations such as Kurdjumov–Sachs. Reasonable agreement with data gathered from molecular dynamics simulations is observed, and the original hypotheses shown to be reasonable.