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Reaction rate predictions of dislocation–precipitate interactions with atomistic simulation

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ABSTRACT

The high strength of many modern engineering alloys can be attributed to the presence of precipitates in the microstructure, which inhibit dislocation motion. Thus, a key step in the quest to comprehensively understand and predict the mechanical behavior of engineering alloys is to develop a sound understanding of dislocation–precipitate interactions. With many features of the dislocation–precipitate interaction being governed by atomic scale processes, atomistic modeling is a valuable tool for improving our understanding. Under this motivation, we will summarize our recent efforts to predict the rate at which a dislocation overcomes a precipitate using atomistic modeling. Specifically, we will focus on the goal of making predictions at timescales and temperatures comparable to typical experiments. Using direct MD simulation as a standard, we first examine the utility of Transition State and Transition Path theories for this problem, using the Finite Temperature String and Transition Interface Sampling (TIS) methods. We find that the TIS approach is the only method that can produce similar predictions to those of direct MD simulations, for the simple reaction coordinate that we have used.