

数学与系统科学研究院

计算数学所学术报告

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报告题目：

Computing Transition Rates of Rare Events in Dislocation Dynamics

邀请人： 明平兵 研究员

报告时间： 2014 年 8 月 22 日 (周五)

上午 10:00-11:00

报告地点： 数学院南楼 702

会议室

Abstract:

We present a numerical method to compute the transition rates including contributions from the potential energy and the entropy effect, of the thermally activated events in dislocation dynamics on the atomistic scale, based on the transition state theory and the string method. The method is applied to the migration of kinks in 30° partial dislocations in silicon. We also present atomistic simulation results on dislocation cross-slip in aluminum at zero temperature, with focus on the dependence of the transition paths and energy barriers on dislocation length and position. Multiple local minimum energy cross-slip paths have been found. A new mechanism with combination of the classical mechanisms has been identified.

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