

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:

Coupled atomistic/continuum  
modeling of brittle crack dynamics

邀请人: 明平兵研究员

报告时间: 2010年1月20日(周三)

下午4:00—5:00

报告地点: 科技综合楼三层311

计算数学所报告厅

Abstract: A coupled atomistic and continuum  
model for numerical simulations of dynamics of  
crystalline solids will be presented. The method

**combines the continuum nonlinear elasto–dynamics model, which models the stress waves and physical loading conditions, and molecular dynamics model, which provides the nonlinear constitutive relation and resolves the atomic structures near local defects. The coupling of the two models is achieved based on a general framework for multiscale modeling – the heterogeneous multiscale method (HMM). An explicit coupling condition at the atomistic/continuum interface is derived.**

**Application to the dynamics of brittle cracks will be presented. Different types of loadings were applied to study the interaction between elastic waves and crack tip behavior. The shock waves were allowed to enter the atomistic region and we also see elastic wave generated in the atomistic region (usually from the crack tip) go into the continuum region while high frequency phonons were absorbed at the interface.**

**The inertia effects of the crack tip were also**

**investigated.**

**欢迎大家参加！**