## 数学与系统科学研究院

## 计算数学所学术报告

## <u>报告人:</u>王绍青研究员 (中国科学院金属研究所)

报告题目:TheoreticalInvestigations on Interface Dynamics<br/>and Precipitation Thermodynamics<br/>of Metals and Alloys<br/>邀请人:曹礼群研究员邀请人:曹礼群研究员报告时间:2009 年 11 月 19 日(周四)<br/>下午 4:00—5:30报告地点:科技综合楼三层 311<br/>计算数学所报告厅

## <u>Abstract:</u>

Knowledge on interface dynamics and precipitation thermodynamics is essential for the

mechanical property design of metals and alloys. The microstructure formation and evolution in alloys are basically determined by precipitation thermodynamics. The dynamic behavior of interface under strain plays a key role for the global mechanical property of the materials. In our recent works, we carried out theoretical investigations on interface dynamics and precipitation thermodynamics of various metals and alloys by molecular dynamics simulation and first-principles calculations. In this talk, I am going to introduce several our recent results on the following two aspects: the dynamic response of symmetrical tilt grain boundaries of metals under shear strain and the crack evolution in bulk nano-metals by molecular dynamics simulations; the structure stability and precipitation dynamics of typical binary alloys by density-functional theory and density-functional perturbation theory calculations.

欢迎大家参加!