2024 年计算材料研讨会

会议程序册

上海大学

Shanghai University

2024 年 7 月 24 号——2024 年 7 月 26 号

本次的会议地点为**上海大学宝山校区乐乎新楼二号楼上善厅**，具体地址是:上海市宝山区上大路 99 号。出行建议:打车请说明到上海大学宝山校区北门，地铁请选择地铁 7 号线上海大学站 2 号口。

会议报告人(姓氏笔画序):

牛晓花 厦门理工学院

朱一超 大连理工大学

张露婵 深圳大学

罗涛 上海交通大学

秦晓雪 上海大学

戴书洋 武汉大学

魏朝帧 电子科技大学

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2024 年 7 月 24 日（星期三）			
全天	报到注册		
2024 年 7 月 25 日（星期四）校本部乐乎新楼二号楼上善厅			
报告时间	报告人	报告题目	主持人
9:00-10:00	牛晓花	A phase field model for the motion of the prismatic dislocation loops by both climb and self-climb	项阳（香港科技大学数学系）
10:00-11:00	朱一超	一回路 690 合金焊接区应力腐蚀开裂长时仿真模型研究	项阳
11:00-12:00	张露婵	Modeling Randomness Effects in High-Entropy Alloys	项阳
午餐及休息			
13:30-14:30	罗涛	Geometry and Local Recovery of Global Minima of Two-layer Neural Networks at Overparameterization	秦晓雪
14:30-15:30	秦晓雪	基于温度的位错动力学模型	秦晓雪
15:30-16:30	戴书洋	质子治疗计划中的优化算法研究	秦晓雪
16:30-17:30	魏朝祯	Structure preserving primal dual methods for Wasserstein gradient flows	秦晓雪
2024 年 7 月 26 日（星期五）			
全天	自由讨论、离会		

A phase field model for the motion of the prismatic dislocation loops by both climb and self-climb

牛晓花

厦门理工学院，应用数学学院

In this talk, we present a phase field model for the dislocation climb motion of prismatic dislocation loops coupling with the dislocation self-climb via vacancy pipe diffusion driven by elastic interactions. The model is set up in a Cahn-Hilliard/Allen-Cahn framework with incorporation of the climb force on dislocations, and is based on the dislocation self-climb velocity formulation established in Ref. (Niu et al, J. Mech. Phys. Solids 2017). Asymptotic analysis shows that the proposed phase field model gives the dislocation climb and self-climb velocity accurately in the sharp interface limit. Numerical simulations of evolution, translation, coalescence and repelling of prismatic loops by self-climb show excellent agreement with discrete dislocation dynamics simulation results and the experimental observation. The simulation results with and without self-climb contribution show the big difference for the prismatic dislocation loops in the evolution time and the pattern.

一回路 690 合金焊接区应力腐蚀开裂长时仿真模型研究

朱一超

大连理工大学，力学与航空航天学院

应力腐蚀（Stress corrosion cracking, SCC）指合金在腐蚀性环境和环境拉伸载荷同时作用下发生断裂的现象。尽管 SCC 对工程管道系统的威胁无处不在，但对 SCC 开展预测研究至少存在以下两方面挑战：a） 极多且相互影响的多物理场因素; b）试验数据获取的经济与时间成本不可承受。为此，本报告尝试建立刻画 SCC 全过程的偏微分方程演化模型。首先以热力学视角对一般 SCC 现象进行了统一建模。随后考虑简化的空间一维模型进而给出裂纹尖端附近应力场的估计式，所得的一维模型其在通用计算机上可在在几秒钟内给出 10 年左右的 SCC 演化过程。经过校准，所提出的方法可用于对压水堆一回路 690 焊接区应力腐蚀寿命进行预测。该模型同时也用于预测石油管路中的不锈钢，以及镁合金心脏支架在各自腐蚀环境下的抗应力腐蚀寿命。

Modeling Randomness Effects in High-Entropy Alloys

张露婵

深圳大学，数学科学学院

High-entropy alloys (HEAs), i.e., single-phase, (nearly) equiatomic multicomponent, metallic materials, have novel mechanical properties (high strength etc). We propose a stochastic Peierls-Nabarro model to understand how random site occupancy affects intrinsic strength. The stochastic Peierls-Nabarro model accounts for the randomness in the composition, characterized by both the standard deviation of the perturbation in the interplanar potential and the correlation length within the spatial compositional distribution. The model predicts the intrinsic strength of HEAs as a function of standard deviation and correlation length of the randomness. We find that compositional randomness induces an intrinsic strength. This approach provides a fundamental explanation to the origin of high strength of HEAs. We also derive stochastic continuum models for HEAs from atomistic models that incorporate the atomic level randomness and the short-range order. These stochastic continuum models theoretically validate the randomness incorporation in our stochastic Peierls-Nabarro model.

Geometry and Local Recovery of Global Minima of Two-layer Neural Networks at Overparameterization

罗涛

上海交通大学，数学科学学院

In this talk, we investigate the geometry of the loss landscape for two-layer neural networks in the vicinity of global minima. Utilizing novel techniques, we demonstrate: (i) how global minima with zero generalization error become geometrically separated from other global minima as the sample size grows; and (ii) the local convergence properties and rate of gradient flow dynamics. Our results indicate that two-layer neural networks can be locally recovered in the regime of overparameterization.

基于温度的位错动力学模型

秦晓雪

上海大学，数学系

位错运动是晶体塑性变形的核心机制之一，对材料的力学性能和可塑性有着重要的影响。随着温度的升高，热振动对位错的影响变得更加显著。高温使位错滑移系统变得更加活跃，使得位错在高温下更容易克服晶格中的能量壁垒，从而降低了 Peierls 应力，进而导致材料的塑性变形增大。本报告提出了一种数据驱动的方法来推导温度依赖的位错动力学模型。我们采用分子动力学（MD）方法并利用嵌入原子势进行模拟。通过 Mori-Zwanzig 正规化方法，推导出广义朗之万方程，以描述位错的动态行为，该方程包括时间依赖的阻尼核函数和随机噪声。基于近似的核函数，我们推导了朗之万类型的一阶模型和二阶模型。通过这些模型，系统研究位错的 Peierls 应力和位错的有效质量，并进一步分析温度对位错的影响。

质子治疗计划中的优化算法研究

戴书洋

武汉大学，数学与统计学院

质子治疗是肿瘤精准放射治疗的先进技术，利用质子束的布拉格峰特性可精准释放能量于肿瘤区域，同时降低正常组织辐射剂量，具有很好的应用前景，但同时由于质子治疗与设备的特性对放疗计划的优化算法提出了更高要求。质子治疗具有很高精度，然而由于射程和设置的不确定性存在，因此在计划过程中需要考虑这些不确定性，需要构建具有鲁棒性的高效算法以避免剂量分布的明显退化。同时，质子治疗系统受到最小跳数(MU)的限制，如果在质子治疗计划优化中不考虑这一限制，将影响剂量分布的质量。然而由于 MU 限制属于非凸约束，因此需要设计适用于非凸优化问题的算法。

Structure preserving primal dual methods for Wasserstein gradient flows

魏朝祯

电子科技大学，数学学院

In this talk, I will present a novel numerical method for a class of continuity equations with concentration-dependent mobilities, which arises widely in applications in biology and material sciences such as tumor growth, swarming dynamics, solid-state wetting/dewetting and thin film surfactant dynamics. This kind of phase field models can be regarded as the gradient flows with respect to some Wasserstein-like transport distances. By leveraging the variational structure, along with the dynamical characterization of the Wasserstein-like transport distance, we construct a fully discrete scheme than ends up with a minimization problem with strictly convex objective function and linear constraint, which can be solved by a primal dual three operator splitting scheme and its accelerated version. Our method has built-in positivity or bounds preserving, mass conservation, and entropy decreasing properties, and overcomes stability issue due to the strong nonlinearity and degeneracy. I will show a suite of simulation examples to demonstrate the effectiveness of our algorithm.