



石墨烯拉伸力学性能温度相关性的分子动力学研究

Temperature dependences of tensile mechanical properties for single graphene sheet: a molecular dynamics study

投稿时间: 2009-1-8 最后修改时间: 2009-10-14

DOI: 稿件编号: 中图分类号: TB323

中文关键词: [单层石墨烯薄膜](#) [拉伸力学性能](#) [分子动力学](#) [温度相关性](#)

英文关键词: [single graphene sheet](#) [tensile mechanical properties](#) [molecular dynamics](#) [temperature dependence](#)

作者	单位	E-mail
韩同伟	同济大学航空航天与力学学院	6twhan@tongji.edu.cn
贺鹏飞	同济大学航空航天与力学学院	
王健	英国贝尔法斯特女王大学	
吴艾辉	同济大学航空航天与力学学院	

摘要点击次数: 50 全文下载次数: 169

中文摘要

采用Tersoff势对扶手椅型(Armchair)和锯齿型(Zigzag)单层石墨烯薄膜在不同温度下(0K-3000K)的单向拉伸力学性能进行了分子动力学模拟, 预测了石墨烯薄膜拉伸力学性能对温度的依赖性, 并比较了不同温度条件下相同几何尺寸的扶手椅型和锯齿型单层石墨烯薄膜拉伸力学性能的差异。结果表明, 石墨烯薄膜的拉伸力学性能和变形机制对温度有强烈的依赖性, 两种不同手性的单层石墨烯薄膜的杨氏模量、抗拉强度、拉伸极限应变均随温度的升高而显著减小。石墨烯薄膜力学性能的各向异性也受温度的影响, 当温度低于600K时, 扶手椅型石墨烯薄膜的力学性能优于锯齿型的, 但当温度超过600K时, 特别是高温时, 扶手椅型薄膜的力学性能的优势逐渐减弱, 甚至低于锯齿型的。

英文摘要

The tensile mechanical properties of the armchair and zigzag single graphene sheets at different temperature (0K-3000K) were investigated using molecular dynamics simulation with Tersoff bond-order interatomic potential. The dependences of the tensile mechanical properties of the sheets on the temperature were predicted and analyzed. The difference of the tensile mechanical properties between armchair and zigzag sheets at different temperature was also studied. Simulation results indicate that the tensile mechanical properties and deformation mechanism of the sheets are strongly dependent on the temperature. The Young's modulus, tensile strength and fracture strain of the two chiral sheets all decrease significantly with increasing temperature. It is also found that the mechanical anisotropy of the sheets is also affected by the temperature. When the temperature is less than 600K, the mechanical properties of armchair sheets are superior to that of zigzag ones. However, when the temperature is more than 600K, this superiority diminishes gradually and even turns into inferiority, especially at high temperature.

[查看全文](#) [查看/发表评论](#)

您是第277975位访问者

版权所有《同济大学学报(自然科学版)》

主管单位: 教育部 主办单位: 同济大学

地址: 上海四平路1239号 邮编: 200092 电话: 021-65982344 E-mail: zrx@tongji.edu.cn

本系统由北京勤云科技发展有限公司设计