力学学报 2007 39 (3(中文)): 320-324 ISSN: 0567-7718 CN: 11-2063/O3

论文

水的汽液界面系统中势能与力的EMD模拟研究

孙杰[1];何雅玲[2];李印实[2];陶文铨[3]

西安交通大学能源与动力工程学院动力工程多相流国家重点实验室，710049[1]

西安交通大学动力工程多相流国家重点实验室, 710049[2]

收稿日期 2006-2-22 修回日期 2006-12-5 网络版发布日期 2007-5-15 接受日期

摘要 分子间势能作用是研究分子界面行为的一个重点所在. 采用平衡态分子动力学模拟(equilibrium molecular dynamics simulation, EMDS)方法，对由水分子构成的汽液界面系统进行了模拟和研究. 分析统计结果符合势能分布在液相区和气相区内存在明显落差的已知结论，并发现不同种力对分子穿越两相区时所起的作用不同，Lennard-Jones(简写L-J)力阻碍分子凝结，而静电力则推动分子凝结并且在合力中起主要作用. 同时，着重对发生相变行为的典型分子进行了追踪和分析，从能量的角度显示了凝结(蒸发)相变过程对应着一个气态(液态)分子由高(低)势能位落入势阱(翻越势垒)的能量降落(抬升)过程.

关键词 分子动力学 凝结 气液界面 势阱 势垒

分类号 0359.1

EMD simulation study on potential and force at liquid-vapor interface system composed of water molecules

Jie Sun Yaling He Yinshi Li Wenquan Tao

Abstract

The interaction of potentials between molecules is important for the molecular interface behavior. The liquid-vapor interface system composed of water molecules is simulated and studied with equilibrium molecular dynamics (EMD) simulation method in this paper. The results agree with the known conclusions that there is a marked fall of potential between the liquid bulk and the vapor bulk. It is also indicated that different types of forces have different effects on the molecules moving across the interface. The L-J force acts as a resistance to condensation while the electrostatic force, which is predominant in the resultant force, acts as motivity. Meanwhile, some typical molecules which participate in the phase-change process, are especially traced. The results show that the process of condensation leads to a drop of the potential energy of a vapor molecule, which falls into the potential well. Correspondingly, the process of evaporation increases the potential energy of a liquid molecule, which gets over the potential barrier.

Key words molecular dynamics condensation liquid-vapor interface potential well potential barrier

DOI:

通讯作者 何雅玲 yalinghe@mail.xjtu.edu.cn