HertZian 软球体系结晶过程中的晶型选择与成核途径

欧阳文泽[1,*]，徐升华[1]，孙祉伟[1]

[1] 中国科学院力学研究所，北京市海淀区北四环西路 15 号，100190

*Email: oywz@imech.ac.cn

本工作采用*NPT*系综下的分子动力学模拟[1]研究了Hertzian软球[2]的结晶过程。我们观察到，是键取向有序性（序参数Q_6）[3]而不是平移有序性（数密度）在结晶过程中起主导作用。结晶形成的晶型由所处的状态点决定。当过冷度较小(温度较高)时，体系趋于结晶成核形成亚稳态的bcc占优势的结构，这可以视为Alexander-McTague机制[4]在起作用。反之，当过冷度较大（温度较低）时，在小的晶核中发现fcc结构占优势。前驱体作为晶体形成的前期相对较有序结构[5]，附着在晶核的外围，其不论体系所处的状态点如何，总是具有高度的bcc对称性结构。以上研究结果可对软核相互作用体系的粒子结晶过程的理解提供新的有益线索。

关键词：分子动力学；结晶；Hertzian球；前驱体

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Polymorph selection and nucleation pathway in the crystallization of Hertzian spheres

Wenze Ouyang[1,*], Shenghua Xu[1], Zhiwei Sun[1]

[1]Key Laboratory of Microgravity(National Microgravity Laboratory), Institute of Mechanics, Chinese Academy of Sciences, No. 15 Beisihuan West Road, Haidian District, Beijing, 100190

The crystallization process of Hertzian spheres is studied by means of molecular dynamics simulations in *NPT* ensemble. It has been observed that the bond orientational ordering (order parameter Q_6) rather than the translational ordering (density) plays a primary role. The crystal polymorphs are determined by the state points. Under the conditions of small supercooling (high temperatures), the system is likely to be nucleated into the crystals that has a preference for the metastable bcc structure, which can be regarded as a manifestation of Alexander-McTague mechanism. In contrast, small nuclei are found to have a preference for fcc symmetry under the conditions of high degree of supercooling. The prestructured precursors that act as the seeds and wet on the nuclei during the nucleation always have a high degree of bcc-like ordering despite different state points. The results above may provide a new clue to the understanding of the crystallization process in core-softened particles.