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论文

［111］晶向银纳米杆结构稳定性的分子动力学模拟

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摘要：

采用分子动力学模拟方法,以超细［111］晶向银纳米杆为研究对象,基于Finnis-Sinclair型多体势,模拟研究了纳米杆在不同温度弛豫过程中的动态平衡变化过程,分析研究了弛豫后银纳米杆的稳态结构变化、平均势能的变化及其在不同时刻结构的演变过程。结果表明温度对［111］晶向银纳米杆结构稳定性将产生重大影响,［111］晶向银纳米杆存在一临界失稳温度,当温度小于临界失稳温度时,体系保持完好线状晶态,当温度大于临界失稳温度小于熔点时,体系坍塌熔化后发生重结晶,截面面积增大,长度明显缩短,随温度增加此特征更加显著,接近熔点时,体系形成由(111)和(100)面围成的多面体且势能最低;当温度大于熔点时,体系变成高度无序的球状团簇。

关键词： 纳米杆 分子动力学 结构 弛豫

Molecular dynamics simulation on the structural stability of the Ag nanorod with ［111］ crystallographic orientation

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Abstract:

The relaxation of a fcc Ag nanorod with ［111］ crystallographic orientation at different temperatures was studied based on the Finnis Sinclair embedded atom potential by a molecular dynamics simulation method. The characteristic of the homeostasis of the Ag nanorod relaxation was demonstrated. The stable structural variation of the Ag nanorod and the optential energy, and the structural evolution of the Ag nanorod at different times were specially studied. The results show that the temperature plays an influential role in the structural stability of the Ag nanorod. A critical temperature of destabilization (Tc) is found in Ag nanorods. When the temperature of the nanorod is less than Tc, the system keeps the intact line form of crystal. When the temperature of the nanorod is higher than Tc and lower than the melting point, the system collapses and fuses, then recrystallizes immediately, and then forms a stable polyhedron bounded by (111) and (100) facets while the temperature nears the melting point. When the temperature of the nanorod is higher than the melting point, the system leads to the formation of disordered spherical clusters.

Keywords: Ag nanorod molecular dynamics structure relaxation

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