纳米铜晶胞体积弹性模量变化规律的分子动力学模拟 Molecular Dynamics Simulation for Variation Relationship of Volume-elasticity Modulus of Crystal Cu with Pressure and Temperature

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关键词： 分子动力学 纳米铜晶胞 体积弹性模量

摘 要： 用分子动力学的方法详细模拟纳米铜晶胞随温度与压强变化的规律，得到了铜晶胞体积弹性模量突变的敏感压强点。模拟结果表明：单晶铜的在压强小于75 GPa时体积弹性模量随温度升高而降低，随压强增大而增大；在压强大于75 GPa时，体积弹性模量随温度升高而增大，随压强增大而减小。 The variation relationship of volume-elasticity modulus of crystal Cu with pressure and temperature was analyzed by molecular dynamics simulation, to gain a sensitive point of pressure value. The results shows the volume-elasticity modulus of crystal Cu decreases as temperature rises, but increases as pressure rises before the point 75?GPa; whereas, exceeding the point, the volume-elasticity modulus of crystal Cu increases as temperature rises, but decrease as pressure rises.

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