

Elastic Constants of Superconducting MgB_2 from Molecular Dynamics Simulations with Shell Model

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Abstract: The elastic constants of superconducting MgB_2 are calculated using a molecular dynamics method (MD) with shell model. The lattice parameters, five independent elastic constants, equations of state (EOS), Debye temperature, and bulk modulus of MgB_2 are obtained. Meanwhile, the dependence of the bulk modulus B , the lattice parameters a and c , and the unit cell volume V on the applied pressure are presented. It is demonstrated that the method introduced here can well reproduce the experimental results with a reasonable accuracy.

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Key words: MgB_2 , elastic constants, shell model, molecular dynamics

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