超离子态冰的弹性异常性质

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Recent shock compression experiments reported phase transitions from solid ice X to SI ice XVIII when temperature was increased to over 2000 K for pressures greater than 100 GPa [1]. The ice X to ice XVIII phase transition, which leads to a structural change in the oxygen sublattice from body centered cubic (bcc) to face centered cubic (fcc), is ascribed to the contribution of extra entropy associated with the fluid-like protons [1].In this work, elastic properties and sound velocities of superionic ice X and ice XVIII are investigated using ab initio molecular dynamics (AIMD) at 200 GPa and temperatures up to 4500 K. The dislocation of protons form their lattice sites leads to the significant elastic softening in ice X with increasing temperature. The phase transition from ice X to ice XVIII leads to an increasing in proton diffusion and elastic softening at 2000 K. We also observed the elastic stiffening with increasing temperature from 2000 to 3000 K in ice XVIII, which is similar to the behavior of some liquids. Above 3000 K, all the elastic constants decrease dramatically. Our study suggests proton diffusion has significant influence on the elastic properties, and the elastic property of superionic ice is different from ordinary solids.

Reference

[1] M. Millot, F. Coppari, J. R. Rygg, A. C. Barrios, S. Hamel, D. C. Swift, and J. H. Eggert, Nature 569, 251 (2019).