ELASTIC AND THERMAL PROPERTIES OF FeNi₃ ALLOY UNDER EARTH'S INNER CORE CONDITIONS

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Summary

The *ab initio* calculations of the electronic structure of crystallographically ordered alloy FeNi₃ at extreme pressures and various temperatures are performed. The elastic and thermal parameters of the compound are studied with the aim to compare the calculated values of sound wave velocities with the observed values of velocities of seismic waves propagating through the Earth's inner core. An attempt is made to estimate the melting temperature of the alloy.