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# Effects of Disordered Atoms and Nanopores on Mechanical Properties of $\beta$-$Zn_4Sb_3$: a Molecular Dynamics Study

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Effects of disordered Zn atoms and nanopores on mechanical properties of $\beta$-$Zn_4Sb_3$ are studied by using the molecular dynamics (MD) method. Due to the influence of disordered Zn atoms in $\beta$-$Zn_4Sb_3$, the elastic modulus decreases from 90.85 GPa to 68.17 GPa, a decrease of 24.96%. The ultimate tensile stress decreases from 18.25 GPa to 9.96 GPa, a decrease of 45.42%. The fracture strain decreases from 32.7% to 20.8%, a decrease of 36.39%. Due to the influence of nanopores, the elastic modulus decreases with growing porosity, and the relationship between the elastic modulus and porosity leads to a scaling law. It seems that the porous radius and porous distribution are also important factors influencing the ultimate tensile stress and fracture strain, in addition to the porosity. However, our simulation results demonstrate that disordered Zn atoms and nanopores reduce the structural stability, dramatically decreasing the mechanical properties of $\beta$-$Zn_4Sb_3$.

**Key words:** Molecular dynamics, mechanical properties, disordered Zn atoms, nanopores, $\beta$-$Zn_4Sb_3$

## INTRODUCTION

Thermoelectric materials have attracted much attention worldwide because they can achieve direct conversion between heat and electrical energy.[1] The conversion efficiency of thermoelectricity-based devices can be measured by the dimensionless figure of merit ($ZT$), which is associated with the electrical conductivity ($\sigma$), Seebeck coefficient ($S$), and thermal conductivity ($k$). It is defined by the following relation:

$$ZT = (\sigma S^2)T/k, \quad (1)$$

where $T$ is the temperature. In fact, in thermoelectricity-based devices, thermoelectric materials are subjected to cyclic thermal loading, which will inevitably reduce their mechanical properties. So, their mechanical stability is of vital importance, and study of mechanical properties of thermoelectric materials plays an important role in thermoelectric commercialization.

$\beta$-$Zn_4Sb_3$ is a high-performing material for thermoelectric applications because of its exceptionally low thermal conductivity, which can be attributed to the disordered Zn atoms in its complex crystal structure.[2–4] It is well known that the discovery of disordered Zn atoms uncovered a highly effective mechanism for reducing thermal conductivity. Meanwhile, the disordered Zn atoms in thermoelectric $\beta$-$Zn_4Sb_3$ also lead to its easily occurring phase transition and structural instability. So, the disordered Zn atoms may be the main reason for its weak mechanics. Recently, experimental studies by Rauwel revealed that nanopores exist in thermoelectric $\beta$-$Zn_4Sb_3$, which uncovers a new porous scattering mechanism to explain the extraordinarily low thermal conductivity of $\beta$-$Zn_4Sb_3$.[5] This, we assume, could also be the reason for the poor mechanical properties of $\beta$-$Zn_4Sb_3$.

The molecular dynamics (MD) method is a well-established and effective alternative to experiment,

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