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Molecular Dynamics Simulation on Mechanics of Mg_2Si Nanofilm

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Molecular dynamics simulation has been carried out to study the mechanical properties of Mg_2Si nanofilm. For the binary thermoelectric material Mg_2Si with antifluorite crystal structure, a modified Morse potential energy function in which the bond-angle deformation has been taken into account is developed and employed to describe the atomic interactions to shed light on its mechanical properties. In the simulation, the radial distribution function of Mg_2Si nanofilm is computed to validate its crystal structure, and the stress–strain responses of the nanofilm are examined at room temperature. It is found that the mechanical properties of Mg_2Si nanofilm are quite different from those of bulk Mg_2Si due to the impact of surface atoms of the nanostructures. The size effect and the temperature effect on the mechanical properties of Mg_2Si nanofilm are discussed in detail.

Key words: Molecular dynamics simulation, mechanical properties, Mg_2Si, nanofilm

INTRODUCTION

In recent years, thermoelectric materials have received extensive attention because of their new power generation applications, in which they can directly convert thermal energy to electricity without any exhaust gases, mechanical vibration, or noise.[1–3] Mg_2Si has been recognized as a potential high-performance thermoelectric material for use in the conversion temperature range of 500 K to 850 K.[4,5] Compared with other intermediate-temperature thermoelectric materials such as PbTe and $CoSb_3$, Mg_2Si has another great advantage, namely that its constituent elements are abundantly available, low cost, and nontoxic. However, for devices made from this thermoelectric material to be more useful in applications, attention should be given to its other basic properties, such as the mechanical properties, which is the focus of the present work. Takeuchi et al.[6] investigated the mechanical properties and plastic deformation mechanisms of Mg_2Si experimentally. Zhou et al.[7] reported the thermal stability, elastic properties, and electronic structures of Mg_2Pb, Mg_2Sn, Mg_2Ge, and Mg_2Si based on the first-principles plane-wave pseudopotential method, the results revealing that Mg_2Si had high structural stability. Baranek et al.[8] studied systematically the effects of the electronic correlation on the charge density distribution, bond structure, lattice parameters, phonon frequencies, and first-order elastic constant by an *ab initio* method. Although much work has been done to study the mechanical properties of Mg_2Si by the first-principles method, little work has been dedicated to the study of size effects and temperature effects on the mechanical properties of Mg_2Si, especially by the molecular dynamics (MD) method. Therefore, further research efforts are still needed for comprehensive understanding of the mechanical properties of Mg_2Si.

Recently, use of nanostructured material has been shown to significantly improve the thermoelectric performance of corresponding bulk materials.[9] Investigation of the mechanical properties of nanofilm is a significant area of materials science,

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