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Effect of Biaxial Strain on Electronic and Thermoelectric Properties of Mg_2Si

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The electronic and thermoelectric properties of biaxially strained magnesium silicide Mg_2Si are analyzed by means of first-principle calculations and semiclassical Boltzmann theory. Electron and hole doping are examined for different doping concentrations and temperatures. Under strain the degeneracy of the electronic orbitals near the band edges is removed, the orbital bands are warped, and the energy gap closes up. These characteristics are rationalized in the light of the electron density transfers upon strain. The electrical conductivity increases with the biaxial strain, whereas neither the Seebeck coefficient nor the power factor (PF) follow this trend. Detailed analysis of the evolution of these thermoelectric properties is given in terms of the in-plane and cross-plane components. Interestingly, the maximum value of the PF is shifted towards lower temperatures when increasingly intensive strain is applied.

Key words: Magnesium silicide, thermoelectric properties, DFT calculations, strained structures

INTRODUCTION

Research on thermoelectricity has attracted new interest in recent decades. By converting heat to electricity, thermoelectric devices enable recovery of waste thermal energy for low-power applications. Thermoelectric devices are typically composed of a plurality of thermoelectric couples connected electrically in series and thermally in parallel. A thermoelectric couple consists of a *p*-type and an *n*-type semiconducting material. Thus, thermoelectric devices have no moving parts, they are reliable and silent, and they do not produce greenhouse gases.[1]

The performance of thermoelectric materials is quantified in terms of the dimensionless figure-of-merit parameter, *ZT*, defined as follows:

$$ZT = \frac{S^2\sigma}{\kappa_{\mathrm{el}} + \kappa_{\mathrm{ph}}}T, \qquad (1)$$

where σ is the electrical conductivity, S is the thermopower, T is the temperature, and κ_{el} and κ_{ph} are the electronic and phononic contributions to the thermal conductivity, respectively. Equation 1 suggests that a key requirement for a good thermoelectric material is a high thermopower and electrical conductivity in the temperature range of interest along with a low thermal conductivity. High-performance thermoelectric materials are usually considered to have *ZT* equal to or greater than one.[2]

Mg_2X (X = Si, Ge, Sn) alloys have been identified as promising advanced thermoelectric materials for use in the temperature range from 500 K to 800 K.[3,4] Compared with other thermoelectric materials operating in the same conversion temperature range, such as PbTe and $CoSb_3$, Mg_2X are environmentally friendly materials, their constituent elements are nontoxic, and they are abundant in the Earth's crust.[5] With this type of materials, it may be possible to extend use of thermoelectricity to large-scale applications rather than being confined to technological niches as is currently the case. Hence, numerous papers have been published on these materials in recent years.[6–11]

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