

Thermoelectric Power of Different Phases and States of Silicon at High Pressure

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The thermoelectric properties of silicon in its high-pressure and metastable (upon decompression) phases in the pressure range up to ~ 25 GPa were investigated. Experimental data were obtained using designed high-pressure cells with sintered diamond anvils. Band-structure calculations based on density functional theory were performed to explain the thermoelectric properties. In particular, it has been established that the nonnegligible positive values of the thermoelectric power S found for the high-pressure “metal” phases of silicon may be well explained by s – d electron scattering. Qualitative agreement between the experimental data and the results of the calculations has been achieved for the known silicon polymorphs named Si-III, Si-V, and Si-XI.

Key words: Thermoelectricity, phases of Si, high pressure, defect-impurity structure of Si

INTRODUCTION

Silicon has remained one of the key materials for microelectronics for several decades, starting from the 1940s. A crucial contribution to the establishment of its electron band structure was made by experiments employing tunable high hydrostatic pressure.¹ In the 1980s, silicon was also suggested to be a promising mechanical material, eventually leading to the advancement of so-called microelectromechanical systems (MEMS).² Nowadays, silicon is the main material used for making miniature machines ranging from microturbines to mirror arrays and fluidic chips. The strong interplay between the electronic and mechanical properties of silicon is used in MEMS devices,² as particularly revealed through the “semiconductor–metal” (S–M) phase transition that may be readily induced by microhardness indentation.^{2,3} In Si-based devices,

local mechanical stresses can drive phase transitions even at negligible load values.^{3,4}

Recently, it was shown that nanostructured silicon has significant potential for use in thermoelectric applications.^{5–7} The dimensionless thermoelectric figure of merit, $ZT = TS^2\sigma/\lambda$, where T is the temperature, S is the Seebeck coefficient, and σ and λ are the electrical and thermal conductivities, respectively, has very low values in the case of bulk silicon, while in silicon nanostructures the ZT parameter may be greatly improved because of optimization of phonon dynamics. Small feature sizes enhance phonon scattering on nanoscale interfaces and thereby can reduce the lattice thermal conductivity by about two orders of magnitude.^{6,7} Recent works have shown that many-fold improvement in ZT at room temperature can be achieved both in membrane Si nanostructures ($ZT \approx 0.4$)⁷ and in Si nanowires ($ZT \approx 0.6$).⁵ Moreover, a value of $ZT \approx 1$ was achieved in case of a nanowire system for temperature of $T = 200$ K.⁶ It is worth noting that one-dimensional (1D) nanowires are limited by a surface

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