

INFLUENCE OF SILICON-BASED COMPOSITE MATERIALS ON SOME THERMOELECTRIC PROPERTIES

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ABSTRACT

In recent years, silicon and its based thermoelectric (TE) materials have attracted attention due to the advantages of low toxicity, low production costs and high stability. In this article, we review recent advances in the synthesis and characterization of silicon-based thermoelectric materials. In the first part of the article, it is shown that a large amount of silicon synthesized by natural nanostructure method, which is one of the new methods, exhibits a very high thermoelectric value of 0.6 zT at 1050 K temperature. In the second part, we consider the synthesis and characterization of Si nanocomposites and silicon-based thermoelectric materials. All of them are synthesized by the melt-spinning technique, which has rapid solidification properties. By this condition, it can be considered that the silicide precipitates are homogeneously distributed in the silicon matrix at any nanoscale size. And in the final part, we show promising new silicon-based thermoelectric composites for general thermo electrics, which exhibit very high power factor even at room temperature.

Keywords: *silicon, thermoelectric, nanocomposite, nanostructuring, melt-spinning.*

INTRODUCTION

In general, most thermoelectric devices focus on generating power from waste heat because they can convert thermal gradients directly into electricity. The efficiency of the thermoelectric device is determined by the temperature gradient across the device, as well as the properties of the thermoelectric material, as the dimensionless value is described by $zT = S^2\sigma T\kappa^{-1}$ [1-3]. Where S is the Seebeck coefficient, σ is the electrical conductivity, T is the absolute temperature, and κ is the total thermal conductivity ($\kappa = \kappa_{\text{lat}} + \kappa_{\text{el}}$, where κ_{lat} and κ_{el} are the lattice and electronic contributions, respectively). In many ways, cheap and non-toxic TE materials that are affordable are needed to expand TE energy production and practical applications. Silicon-based materials are abundant in supply because they make up most of the Earth's surface, making them useful for use in TE electricity generation. For decades, various Si-based

TE materials such as Si–Ge alloys and Mg₂Si have been developed with a maximum zT value of around unity at 1100 K [4-6]. Analogously, it is informed that some metal silicides have potential to be a good TE material. One of the top metal silicides is Mg₂Si. It has been established that Mg₂(Si,Sn) displays n-type characteristics with a zT value of over unity at 700 K [7-8]. For p-type metal-silicide TE materials, bigger manganese silicides have been improved, in which the topmost zT value of 0.7 at 800 K has been confirmed. Even though bulk Si exhibits nice electrical properties, its κ_{lat} is immoderate ($>140 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ at 300 K for a non-doped alone crystal), yielding a low zT value of ~ 0.02 at maximum at 300 K [9,10]. Accordingly, recent research on Si-based TE materials has concentrated on methods to lessen κ_{lat} . In recent years, significant improvements in zT in different traditional TE materials have been attained, particularly via considerable methods for the minimization of κ_{lat} including mixture scattering, rattling, lone-pair electrons and nanostructuring [11-16]. Nanostructuring allow κ_{lat} reduction while maintaining high some electrical properties. Additionally to Si, many metal silicides are considered developed TE materials because of its low toxicities and high chemical stabilities.

METHODS

In many cases nanostructured TE materials are traditionally synthesized by grinding the materials into small-sized particles and consolidating these materials entering to polycrystalline bulks. Nevertheless, synthesizing fine nanostructured bulk Si by this method is hard because Si nanopowders are easily oxidized within the grinding act. Therefore, in this work has proposed an alternative synthesis of nanostructured bulk Si by precipitating nanoscale particles in the Si based [17-19]. This usually made nanostructures and effectively prevents oxidation. As we can see from the Si-P phase diagram, the solubility of P in Si is mainly temperature-dependent. At large temperature, a small percentage of P can dissolve contains Si, and at room temperature, nearly no P dissolves. Therefore, when a thaw of highly P-doped Si cools from the α -phase region (Figure 1a), it is expected that P-rich precipitates form in the Si matrix. By using this method successfully synthesized nanostructured bulk Si. And also it confirmed that two types of precipitates form in the Si matrix: semi-coherent plate-shaped precipitates of several dozen nanometers and coherent spherical-shaped precipitates of a little nanometers in size, as shown in Figure 1b–d. Transmission electron microscopy/energy-dispersive X-ray spectroscopy analysis realize that the precipitates are Si–P binary compounds.

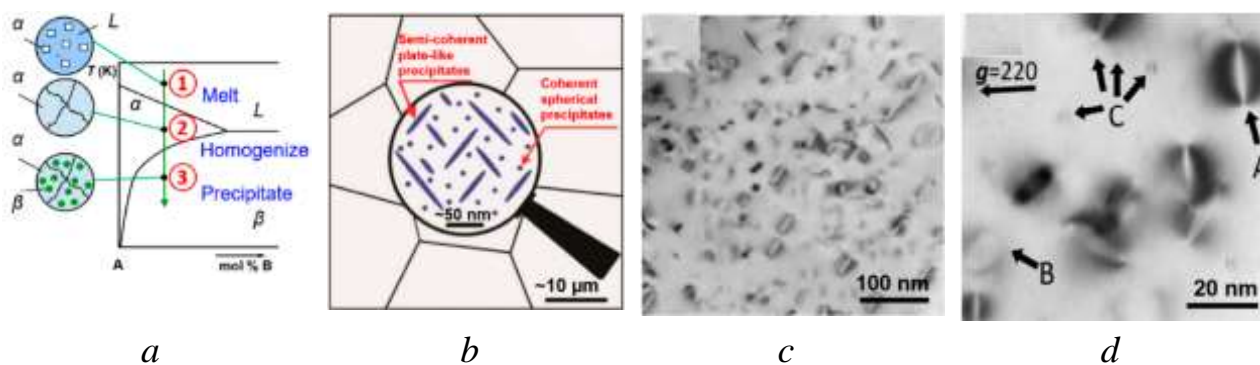


Figure1. (a) Precipitates naturally form when the melt cools from the α -phase region in a binary phase diagram. (b) Micro- and nanoscale schematics of a nanostructured bulk material containing various types of precipitates. (c) Low- and (d) high-magnification bright-field transmission electron microscopy (TEM) images of nanostructured bulk Si, showing the homogeneous distribution of nanoscale precipitates in the Si matrix. Contrast shows strain arising from the precipitates. In (d), the arrows A and B indicate plate-like precipitates along (high contrast) and perpendicular (lesser contrast) to the electron beam, respectively.

RESULTS

We can see at the eutectic composition, nanocomposites with homogeneous distributions of secondary phases in the primary-phase matrix can be obtained. Several metal silicide's might form such nanoscale precipitates in Si matrices because they have a pseudo-binary eutectic point with Si. So, as summarized in Figure 2, the structural characteristic of the secondary phase, i.e., nano-lamellar or nano-dot, depends on the position of the eutectic point. For example, among various metal silicides, CrSi_2 , CoSi_2 , Si_2Sb and TiSi_2 have eutectic points with Si at intermediate dopant concentrations, while VSi_2 has a eutectic point with Si at low V concentrations.

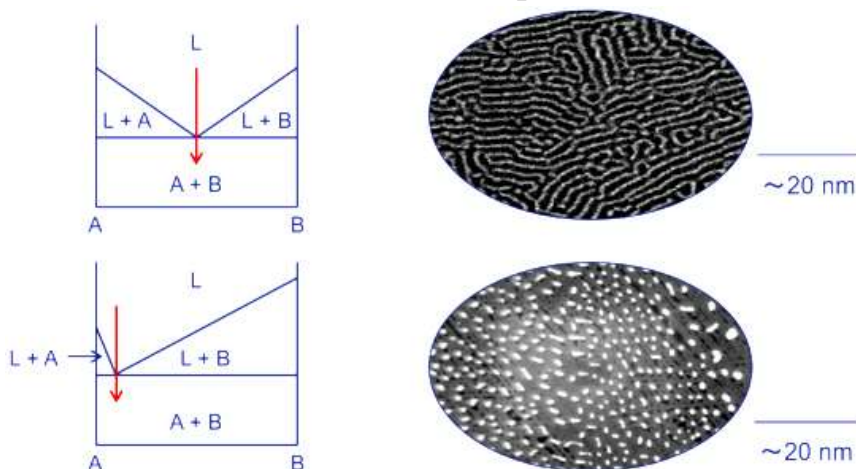


Figure2. Relationship between phase diagram and nanostructure. According to the position of the

eutectic point, nano-lamellar or nano-dot structure can be obtained by melt-spinning (MS).

Figure 3 we can see scanning electron microscopy (SEM) images of the nano-lamellar structures obtained by MS at the eutectic points between Si and different metal silicides. All composites comprised two phases, i.e., white and dark areas corresponding to the metal silicide and Si matrix, respectively.

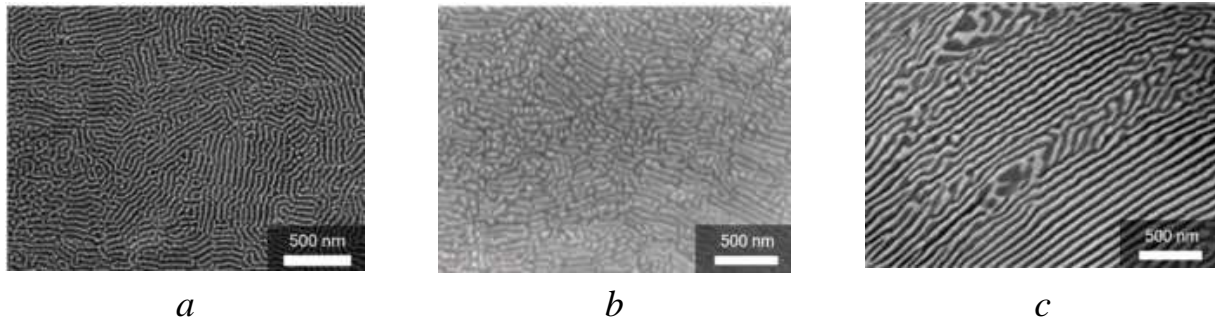


Figure 3. Scanning electron microscopy (SEM) images of nano-lamellar structures obtained by MS at the eutectic points between Si and metal silicides: (a) Si-CrSi₂, (b) Si-CoSi₂, and (c) Si-TiSi₂.

DISCUSSION

It has discovered that YbSi₂- δ exhibits a high power factor of $2.2 \text{ mW} \cdot \text{m}^{-1} \cdot \text{K}^{-2}$ at room temperature. Because of the mixed valence behavior of Yb, YbSi₂- δ has an extraordinarily high S value despite its metallically high σ . And also, it has demonstrated that the power factor of YbSi₂- δ can be improved by substituting Si by Ge. It should be mentioned as an explanation the substitution gradually changed the structure from A1B₂ type with random defects to Th₃Pd₅ type with ordered defects, reducing the level of disordered defects, as shown in Figure 4.

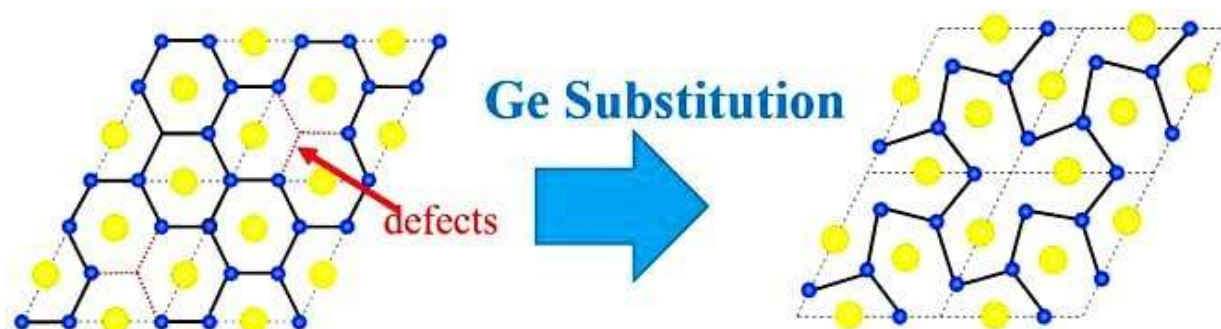


Figure 7. Schematic of crystal structure of YbSiGe projected along the c axis, showing a structural transition from the disordered A1B₂-type structure to the ordered Th₃Pd₅-type structure. Yellow and blue balls represent Yb and Si/Ge, respectively.

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The composition dependences of the Hall mobility μ_H , Hall concentration n_H , and $\sigma (=e \cdot \mu_H \cdot n_H)$ values the n_H values decreased with the increasing Ge content, possibly because of the reduced density of states near the Fermi stage. Also, the valence states of Yb in the compounds tended to decrease from 3^+ to 2^+ with the increasing Ge content, which may reduce the number of conduction-band electrons, thus reducing n_H . Meanwhile, μ_H values increased considerably with the increasing Ge content, possibly because of changes in the band structure, reductions in electron scattering, and the removal of disordered defects in the Si sub-lattices via the structural transition discussed above. Based on the results of n_H and μ_H , the electrical conductivity $\sigma (=e \cdot \mu_H \cdot n_H)$ was increased approximately linearly with the Ge content.

CONCLUSION

In this review, recent research toward the development of high-efficiency eco-friendly Si-based TE materials was summarized. The nanoscale precipitates reduce κ_{lat} without significantly affecting the electron transport properties, thus enhancing zT . In addition to this natural nanostructuring procedure, our group has proposed the rapid-solidification MS method to synthesize Si–metal silicide nanocomposites. At the eutectic composition of Si and a given metal silicide, a eutectic structure with a homogeneous dispersion of metal silicides in the Si matrix can be obtained. Furthermore, with varied cooling rates, the eutectic structure feature size can be controlled, that is, higher cooling rates correspond to smaller sizes, as demonstrated in the Si– VSi_2 system. Finally, it has discovered a promising high-power-factor TE metal silicide, $YbSi_2$. For this reason, because of the mixed valence state of Yb, this metal silicide exhibits a large S with a metallicly high σ , yielding a high room-temperature power factor. Furthermore, the power factor can be enhanced by the substitution of Ge for Si.

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