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The Maximums of the Seebeck Coefficient and Figure of Merit of Thermoelectric

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Abstract

This article provides an assessment of the maximum values of the most important thermoelectricparameters of materials - the Seebeck coefficient and the figure of merit. Based on the formulas known from the literature that interconnect the thermoelectric parameters (effective mass and mobility of charge carriers, the Seebeck coefficient, temperature), the function of the specified coefficient is obtained. To estimate the maximum of the Seebeck coefficient and the figure of merit, it is sufficient to study this function for an extremum by differentiating it be used. The data we obtained can be used to analyze the experimental data of those works in which, for certain reasons, the extremums of the specified thermoelectric parameters are not given.

Keywords: Thermoelectric, Seebeck Coefficient, Figure of Merit

1. Introduction

The Seebeck effect is that if the ends of a metal or semiconductor sample are at different temperatures, thermal diffusion will occur. Since the thermal motion of electrons at the hot end is faster than at the cold end, more electrons will move from the hot end to the cold end than in the opposite direction. The current resulting from this diffusion causes the cold end to become negatively charged relative to the hot end, causing a voltage to develop between the two ends. The thermal diffusion voltage U is proportional to the temperature difference between the two ends (T1 - temperature at the hot end, T2 -temperature at the cold end): U=S(T1-T2), where the proportionality coefficient S is called the Seebeck coefficient. The Seebeck effect is used in voltage and temperature sensors, gas pressure meters, thermal electric generators, light intensity controllers and in many other equipments. They are used in navigation systems, generators, spacecraft, solar energy converters, heating equipment, oil and gas processing plants, thermal energy converters. The Seebeck coefficient often has extreme values, in many cases - both minimum and maximum [1-31]. This is demonstrated in Figs (1-3) based on literary and our data.

The data on Bi2S3–xTex and CrxMo1-x were taken from the literature we studied the alloy SixGe1-x. The st [udied samples were produced by vacuum hot pressing of powders obtained from zone melting ingots [5,6].

In this paper, the extremums of the Seebeck coefficient and figure of merit are considered. For practical purposes, it is of interest to determine the maximums of these this characteristic.

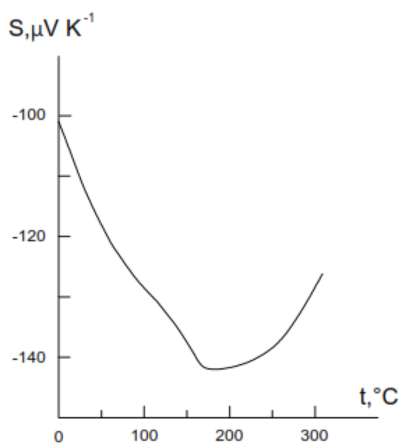

Figure 1: S – T Dependence for $Bi_2S_{3-x}Te_x$ from [5]; (the Value of x is Notspecified)

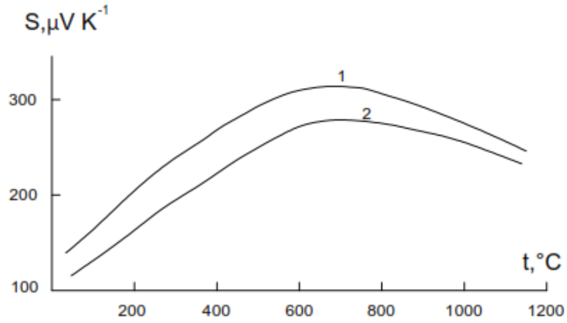

Figure 2: S – T Dependence for Si_xGe_{1-x}: x=0.3 (1) and 0.17 (2)

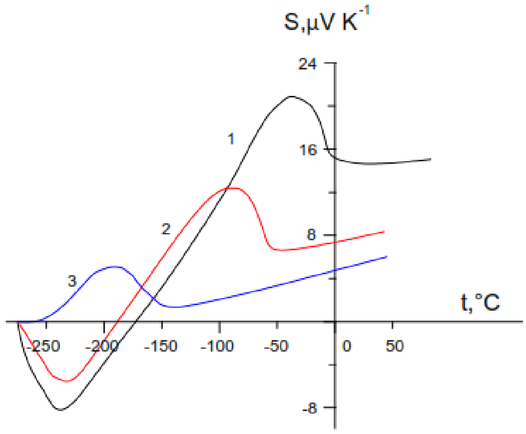

Figure 3: S – T Dependence for Cr_xMo_{1-x} from [6]: x=0.03 (1), 0.07 (2) and 0.15 (3)

1.1. Experimental

The composition of alloys significantly impacts their mechanical properties. For instance, the addition of alloying elements can alter strength, ductility, and corrosion resistance. In additive manufacturing, the choice of alloy is crucial as it determines how the material responds to the thermal cycles of the process. Techniques such as heat treatments and hot isostatic pressing can enhance the mechanical properties by reducing residual stresses, improving microstructure, and eliminating defects. The build environment, including temperature and atmospheric conditions, can influence oxidation and contamination, indirectly affecting mechanical properties. Controlling these conditions is crucial for ensuring the quality and performance of the alloys. Since the previous section mainly describes literature data, here we will describe only the procedure for preparing of SiGe samples.

To create a thermoelectric module, n- and p-type Si0.7Ge0.3 alloys containing alloying substances with a concentration of 3.2·1026 m-3 were fabricated by the vacuum hot-pressing method. Massive wastes of Si and Ge were crushed with a steel rod and sieved through a (with 0.2 mm cells) sieve. Then it was loaded into the mill chamber (“REC” PM-100 SM) and ground for 20-25 hours. The powder grain size was assessed using an optical microscope (Nicon) and an X-ray diffractometer (DRON-3M). The disperced Si0.7Ge0.3 alloy powder produced in the indicated mode consisted mainly of Si and Ge grains of size 60–80 nm. The resulting powder was pressed in a high-temperature vacuum induction pressure chamber at a temperature of 1200-1320°C and a pressure of 480 kg·cm-2 for 20-30 minutes. The matrix and punches are made of highstrength graphite. From the obtained briquettes, profiled samples were cut out on a diamond-cutting disk device. Photo of briquette is shown in Fig.4. Graphite switching plates were attached to the ends of the alloy branches. The switched sample was placed in the vacuum chamber of an induction furnace, and probes were placed in its switching plates to measure the temperature and electromotive force. One side of the module was heated by a flame generated by gas combustion, which directly hit the surface of the module. On the other side, the module was cooled by running water. Chromel-alumel thermocouples were placed on the hot and cold ends of the module. The monolithic thermoelectric module's cold side electrical insulation node was fabricated using AlN and graphite plates. Both of them are thermomechanically combined with SiGe alloys in a wide temperature range, which is very important for creating a thermostable. Figure 5 shows photo of module from 16 branches. 4 n- and p-type alloy plates (2 n-type and 2 p-type) were taken to make a mini monolithic thermoelectric module containing 16 branches. They were arranged in n-p-n-p order.

Figure 4: Photo of Briquette Compacted from Ultra Dispersed $Si_{0.7}Ge_{0.3}+P_{0.5}$ Alloy Powder at 1300°C

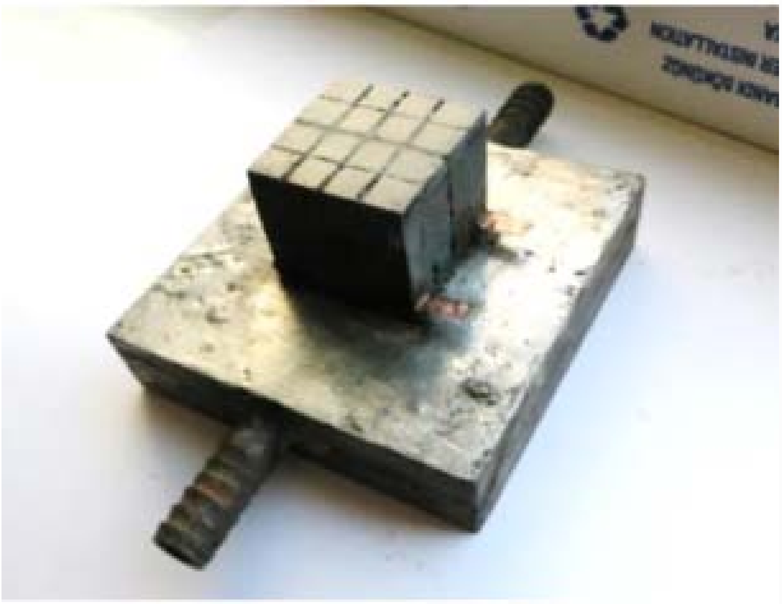

Figure 5: Photo of Thermoelectric Module Connected to Water Cooler

2. Results and Discussion

To compile an expression for S, formulas known from the literature (Snyder et al. 2022) relating the absolute temperature (T), effective mass (m*), and concentration of charge carriers (n) are used

$$S \sim \frac{m^{*}T}{n^{2/3}}, \; m^{*} \sim \left(\frac{n^{2/3}}{T}\right)\left\{\frac{\left[e^{(S_r-2)}-0.17\right]^{2/3}}{1+e^{-5(S_r-S_r^{-1})}}+\frac{S_r}{1+e^{5(S_r-S_r^{-1})}}\right\}, \; S_r=\frac{q_e}{k_B}|S|\approx 11605|S|$$

reduced Seebeck coefficient (qe – elementary charge, kB – Boltzmann's constant). By combining these formulas, we obtain the expression:

$$f(S) \sim \left\{\frac{\left[e^{(11605|S|-2)}-0.17\right]^{2/3}}{11605|S|\left[1+e^{-5(11605|S|-8.617\cdot 10^{-5}|S|^{-1})}\right]}+\frac{1}{1+e^{5(11605|S|-8.617\cdot 10^{-5}|S|^{-1})}}\right\}. \quad (1)$$

Figure 6 shows the dependence f(S) – S and f'(S) – S, on which the extremes are clearly expressed.

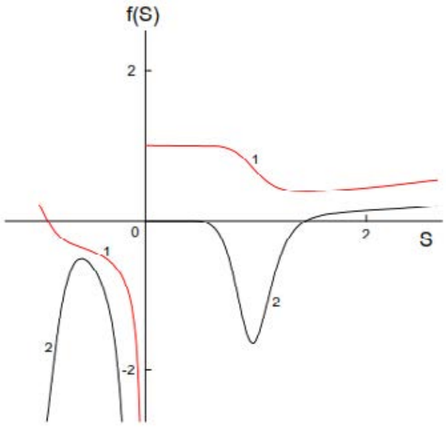

Figure: 6 Dependences f(S) – S (1) and f'(S) (2) According to Eq. (1)

After of this, it is easy to determine the maximum figure of merit ZT=(σS2) T/k, where σ is specific electrical conductivity and k is thermal conductivity coefficient (the sum of its electronic and lattice components). Using the Wiedemann-Franz law we will have $ZT \sim S^2$ and $(ZT)_{max} \sim (S^2)_{max} \sim S_{max}$.

The presented approach can be used to predict the maximum values of the considered thermoelectric parameters in cases where they are not revealed due to the limitation of their measurement range.

3. Conclussion

The maximum values of thermoelectric parameters of materials - Seebeck coefficient and figure of merit are estimated. Based on the formulas known from the literature, which interconnect the thermoelectric parameters, the function of the mentioned coefficient is obtained. To estimate the maxima of the Seebeck coefficient and the figure of merit, it is sufficient to study this function for an extremum by differentiating it. The obtained data can be used to analyze the experimental data of those works in which, for some reason, the maxima of the specified thermoelectric parameters are not given.

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Footnote:

Having estimated the maximum Seebeck coefficient, we can also consider the issue of maximization the power factor PF≡σS2=nqeμS2 (μ - mobility of charge carriers). Using the equations from [27,28] we get:

$$\mu \cong \left(\frac{m^*}{m_0}\right)^{-3/2} \mu_W,$$

$$\frac{m^*}{m_0} \sim \left(\frac{n^{2/3}}{T}\right)\left\{\frac{3\left[e^{(S_r-2)}-0.17\right]^{2/3}}{1+e^{-5(S_r-S_r^{-1})}}+\frac{S_r}{1+e^{5(S_r-S_r^{-1})}}\right\},$$

$$\mu_W \sim \left\{\frac{e^{(S_r-2)}}{1+e^{-5(S_r-1)}}+\frac{\frac{3}{\pi^2}S_r}{1+e^{5(S_r-1)}}\right\} \rightarrow$$

$$\rightarrow PF \sim T^{3/2}\left\{\frac{\left[e^{(S_r-2)}-0.17\right]^{2/3}}{1+e^{-5(S_r-S_r^{-1})}}+\frac{S_r}{1+e^{5(S_r-S_r^{-1})}}\right\}\left\{\frac{e^{(S_r-2)}}{1+e^{-5(S_r-1)}}+\frac{\frac{3}{\pi^2}S_r}{1+e^{5(S_r-1)}}\right\}\left\{\frac{3\left[e^{(S_r-2)}-0.17\right]^{2/3}}{1+e^{-5(S_r-S_r^{-1})}}+\frac{S_r}{1+e^{5(S_r-S_r^{-1})}}\right\}^2,$$

where μ_W is weighted mobility [27,28].

To determine (PF)max, the function f(T, m*, μw)=f(T, S) should be considered using the Lagrange multiplier method. This issue will be discussed in the continuation of this communication.

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