Some considerations towards design and optimization of segmented thermoelectric generators

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Abstract

This paper presents some considerations about segmented thermoelectric generators. The equations and the important quantities (such as the compatibility factor or the maximum of the reduced efficiency) that permit to determine wether it is interesting or not to segment thermoelectric materials together are presented. Results are given for several p-type and n-type thermoelectric materials. The example of a leg with three segments is then investigated.

Introduction

The aim of almost all the devices designers is obviously to achieve high efficiency. Thermoelectricity is not an exception to this rule that is why a lot of studies are made in order to improve the efficiency of thermoelements [1,2].

As no single thermoelectric material presents high figure of merit over a wide temperature range, it is therefore necessary to use different materials and to segment them together in order to have a sandwiched structure [3,4]: in this way, materials are operating in their most efficient temperature range. Even if the thermoelectric figure of merit z is an intensive material property of prime importance, it is not the only one: indeed the expression of the reduced efficiency involves another parameter called the compatibility factor [5], which must be considered and controlled to determine the relevance of segmentation.

After recalling the exact expression of the reduced efficiency, approximations based on polynomials expansion are given. Not only the reduced efficiency but also the compatibility factor are then plotted for different n-type and p-type elements such as skutterudite. Thanks to these considerations, the design of the segmented thermoelectric device is investigated in order to optimize the efficiency and once the materials chosen, to determine the best operating conditions.

Equations with significant variables and quantities

The relative current density [5] is the ratio of the electric current density to the heat flux by conduction:

$$u = J/\lambda \nabla T \tag{1}$$

The variation of u is governed by the heat equation and then satisfies the following differential equation:

$$\frac{d(1/u)}{dT} = -\frac{1}{u^2}\frac{du}{dT} = -T\frac{d\alpha}{dT} - u\,\rho\,\lambda \tag{2}$$

where the Seebeck coefficient, the resistivity and the thermal conductivity can be functions of temperature.

The reduced efficiency is defined as the power produced divided by the power supplied to the system:

$$\eta_r = \frac{E\cdot J}{-\nabla T\cdot J_S} = \frac{E\cdot J}{-\frac{\nabla T}{T}\cdot q} = \frac{\alpha\,J\cdot\nabla T - \rho\,J^2}{\frac{\lambda}{T}(\nabla T)^2 + \alpha\,J\cdot\nabla T} \tag{3}$$

It could be expressed as a function of u and of the thermoelectric figure-of-merit z:

$$\eta_r(u) = \frac{u\frac{\alpha}{z}\left(1 - u\frac{\alpha}{z}\right)}{u\frac{\alpha}{z} + \frac{1}{zT}} = \frac{1 - u\frac{\alpha}{z}}{1 + \frac{1}{u\alpha T}} \tag{4}$$

The aim is to optimize this quantity. The value of the relative current density which gives the largest reduced efficiency is noted s and called the thermoelectric compatibility factor:

$$s = \frac{\sqrt{1+zT} - 1}{\alpha T} \tag{5}$$

If the compatibility factors of materials which must be segmented together differs by a factor 2 or more, a value of the relative current density can not be suitablefor both materials and it is obvious that the working point could not be optimum for the both together. In that case, the segmentation is not useful and does not permit to increase the efficiency.
Then the two quantities on which the attention is focused now are the thermoelectric compatibiliy factor and its evolution versus temperature and the reduced efficiency and its evolution as a function of the relative current density.

Thermoelectric compatibility factor

Before performing calculations on the exact expression of the compatibility factor, it is also interesting to find an approximate value of this factor for small and large values of zT.

- For small zT, let consider $\varepsilon = zT$,

$$s = \frac{\sqrt{1+\varepsilon} - 1}{(\alpha/z)\,\varepsilon} \underset{\varepsilon\to 0}{=} \frac{z}{\alpha}\left(\frac{1}{2} - \frac{1}{8}\varepsilon + o(\varepsilon)\right) \underset{\varepsilon\to 0}{\approx} \frac{z}{2\alpha} = \frac{\alpha}{2\lambda\rho}$$

- For large zT, let consider $\zeta = zT$,

$$s = \frac{z}{\alpha}\left(\frac{(1+\zeta)^{1/2} - 1}{\zeta}\right) \underset{\zeta\ grand}{=} \frac{z}{\alpha}\left(\frac{1}{\zeta^{1/2}} - \frac{1}{\zeta} + o(\frac{1}{\zeta})\right) \underset{\zeta\ grand}{\approx} \frac{z}{\alpha}\zeta^{-1/2} = \frac{\alpha}{\lambda\rho\sqrt{zT}}$$

The expression of the compatibility factor given by the equation (5) is used to plot its evolution versus temperature for different thermoelectric materials. The curves obtained are represented for n-type thermoelectric materials on the figure 1 (respectively for p-type thermoelectric materials on the figure 2).

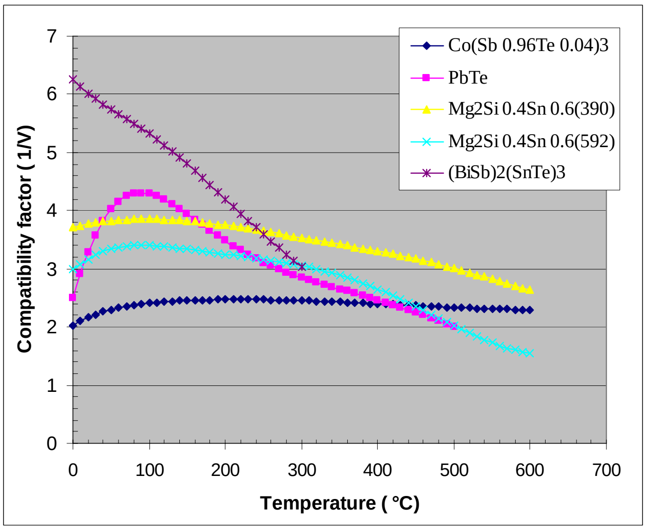

Figure 1: Compatibility factor versus temperature for n-type materials

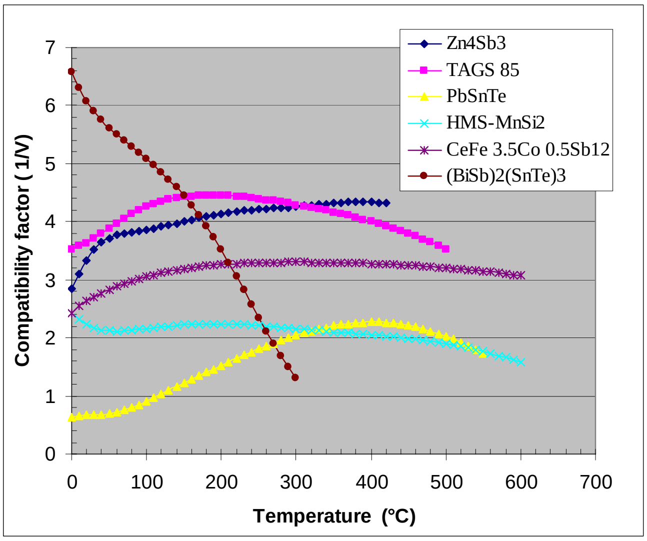

Figure 2: Compatibility factor versus temperature for p-type materials

Maximum of the reduced efficiency

The maximum of the reduced efficiency is obtained when the relative current density is equal to compatibility factor. The expression of the maximum of the reduced efficiency is then:

$$\max \eta_r(u) = \eta_r(s) = \frac{1 - s\frac{\alpha}{z}}{1 + \frac{1}{s\alpha T}} = \frac{1 - \left(\frac{\sqrt{1+zT}-1}{\alpha T}\right)\frac{\alpha}{z}}{1 + \frac{1}{\left(\frac{\sqrt{1+zT}-1}{\alpha T}\right)\alpha T}} = \frac{\sqrt{1+zT}-1}{\sqrt{1+zT}+1} \quad (6)$$

It is also interesting to find an approximate value of this factor for small and large values of zT.

- For small zT, let consider $\varepsilon = zT$

$$\max \eta_r(u) = \frac{\sqrt{1+\varepsilon}-1}{\sqrt{1+\varepsilon}+1} \underset{\varepsilon \to 0}{=} \frac{1}{4}\varepsilon - \frac{1}{8}\varepsilon^2 + o(\varepsilon)$$

$$\max \eta_r(u) \underset{\varepsilon \to 0}{\approx} \frac{1}{4}\varepsilon = \frac{1}{4} zT$$

- For large zT, let consider $\zeta = zT$,

$$\max \eta_r(u) = \frac{\sqrt{1+\zeta}-1}{\sqrt{1+\zeta}+1} \underset{\zeta\ grand}{=} 1 - 2\zeta^{-1/2} + 2\zeta^{-1} + o(\zeta^{-1})$$

$$\max \eta_r(u) \underset{\zeta\ grand}{\approx} 1 - 2\zeta^{-1/2} = 1 - 2\sqrt{zT}$$

The expression of the maximum of the reduced efficiency given by the equation (6) is used to plot its evolution versus temperature for different thermoelectric materials. The curves obtained are represented for p-type thermoelectric materials on the figure 3 (respectively for n-type thermoelectric materials on the figure 4).

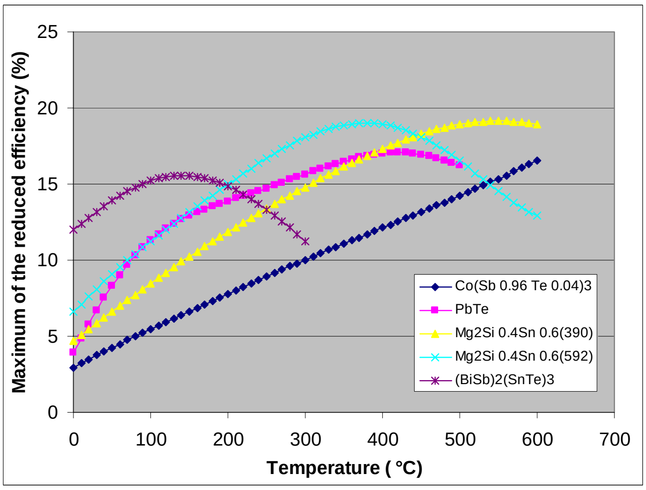

Figure 3: Maximum of the reduced efficiency versus temperature for n-type materials

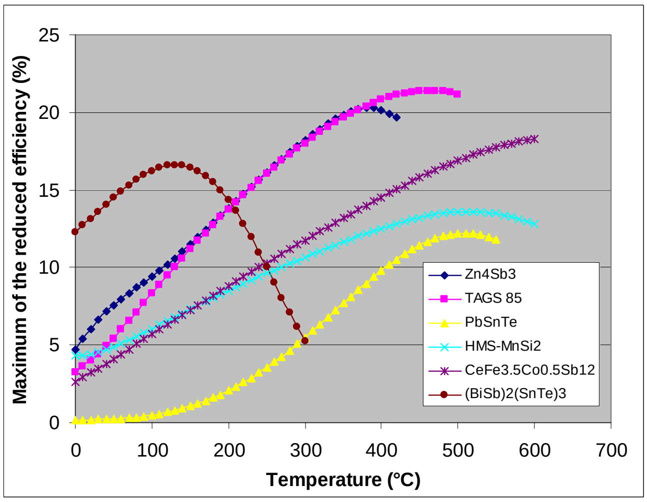

Figure 4: Maximum of the reduced efficiency versus temperature for p-type materials

Reduced efficiency

The reduced efficiency is expressed as a function of the relative current density u, the thermoelectric figure-of-merit z and the temperature T and its expression is given by the equation (4). Up to now, the attention is focused on the evolution of the reduced efficiency as a function of the relative current density.

On the figure 5, the curves are plotted for the example of the three following different p-type materials:

- (BiSb)2(SnTe)3 at 100 °C, at this temperature : $(\alpha, z, \zeta) = (204.44; 2.4784; 0.92436)$
- Zn4sb3 at 300°C, at this temperature : $(\alpha, z, \zeta) = (182.45; 1.9054; 1.00887)$
- CeFe4Sb12 at 550°C, at this temperature: $(\alpha, z, \zeta) = (166.68; 1.2751; 1.0494)$

The interest of considering these three curves for these three p-type materials will be developped further.

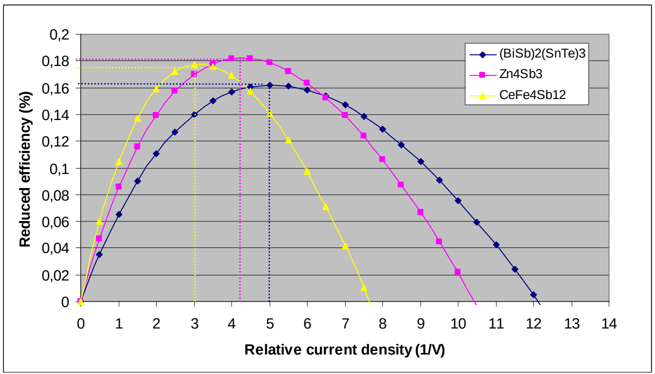

Figure 5: Reduced efficiency versus relative current density for some p-type materials

The evolution of the reduced efficiency versus the relative current density always presents the same shape as a “bell”. The maximum of the reduced efficiency is achieved when the relative current density is equal to the compatibility factor and the curve crosses the axe of abscissa for a value of the relative current density of z/α. The figure 5 permits to summarize all the important values in the following table I.

Table I : Some values for some p-type materials

Material	Temperature	Max η_r	s (1/V)
(BiSb)2(SnTe)3	100°C	~16%	~5 V^{-1}
Zn4Sb3	300°C	~18%	~4,25 V^{-1}
CeFe4Sb12	550°C	~18%	~3 V^{-1}

These informations could be confirmed by figure 6 extracted from the curves of the figure 2.

Nota bene: it is very interesting to plot the evolution of the reduced efficiency as versus the relative current density. Indeed, as the relative current density does not vary a lot in the leg of the thermoelement, the figure 5 permits to confirm the results of the figure 6 and to determine if it is interesting or not to segment thermoelectric materials together.

Indeed, in the figure 5, it is obvious that the thermoelectric material have their maximum of reduced efficiency for values of the relative current density which are very close to each other.

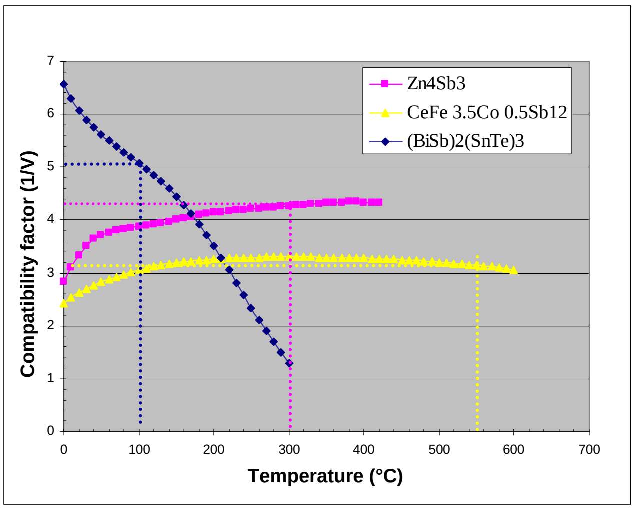

Figure 6: Reduced efficiency versus relative current density for some p-type materials

The relative current density which is good for the three thermoelectric materials (i.e. that permits to the three thermoelectric materials to work in the case of a good reduced efficiency) does exist and is contained between 3 and 5.

As a general rule, the closer the lower and upper bounds are, the more efficient the segmentation is. On the opposite, it is completely useless to segment two materials together whose interval presents a too large range.

For instance, it is not interesting to segment the p-type thermoelectric material SiGe (usually used for temperatures superior to 600°C) with the materials previously cited. Indeed its « bell-shaped » curve representing the reduced efficiency presents a narrow basis and cut the axe of abscissa for a value of the relative current density which is about 2 V^{-1} (against 12 V^{-1}, 10.5 V^{-1} and 7.5 V^{-1} for the three other thermoelectric materials) and the compatibility factor is about 1 V^{-1} (against 5 V^{-1}, 4.25 V^{-1} and 3 V^{-1}).

Remark: a priori it could be a good idea to represent the reduced efficiency as a function of the two variables u and T which will give a surface in 3D as the one represented on the figure 7.

But the interpretation is less easy than with the 2D curves previously plotted. It is really easier to use the compatibility factor represented as a function of temperature (figures 1 and 2) and the maximum of the reduced efficiency of temperature (figures 3 and 4) and the reduced efficiency as a function of the relative current density (figure 5).

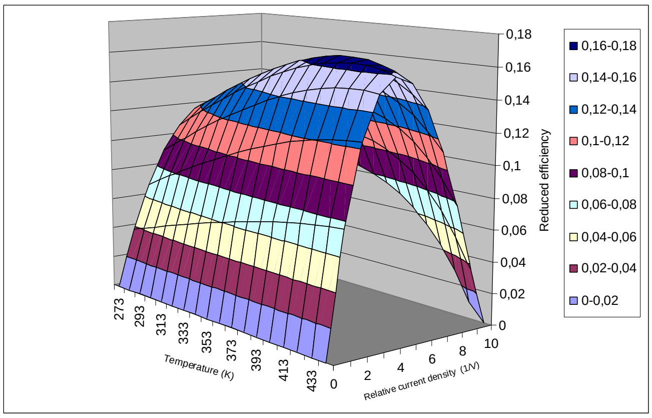

Figure 7: Reduced efficiency
versus temperature and relative current density

Example of a segmented leg

The three thermoelectric materials previously studied are chosen to constitute the leg. The different significant quantities are then represented. First of all, the relative current density going through the whole leg and the compatibility factor are represented as functions of temperature in the figure 8.

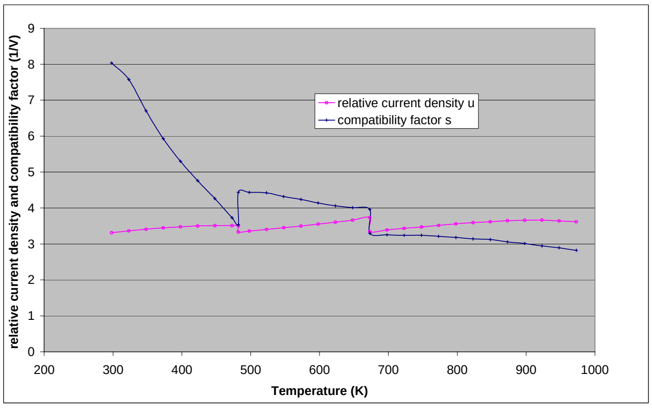

Figure 8: Relative current density and compatibility factor
versus temperature for the segmented p-leg

The variations of the relative current density are not important (from 3,3 V^{-1} to 3,75 V^{-1} that correspond to a relative variation less than 20%). The abrupt changes correspond to the interface of the thermoelectric materials. For (BiSb)2(SnTe)3, the value of the relative current density is a little bit far from the value of the compatibility factor but for Zn4Sb3 and CeFe4Sb12, it is really close. One could expect that for the first segment constituted by (BiSb)2(SnTe)3, the reduced efficiency is far from the maximum reduced efficiency but quasi maximum for the two other ones. Let check this remark by plotting the reduced efficiency compared to the maximum reduced efficiency (see figure 9). The real reduced efficiency varies from 12% to 21 % whereas the maximum of the reduced efficiency varies from 14% to 21%. Obviously, the first segment has a real reduced efficiency lower thant the maximum one but results are very good for the two other segments.

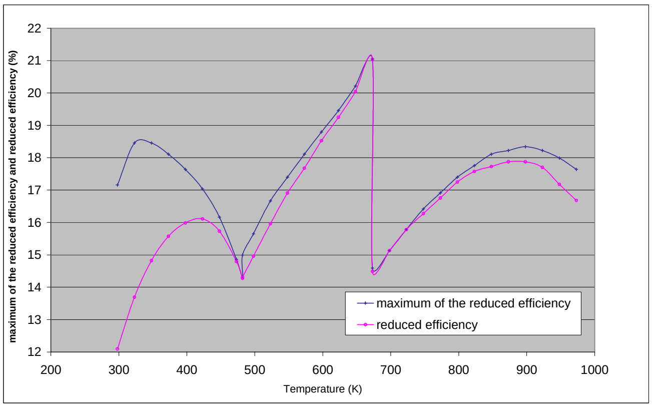

Figure 9: Maximum reduced efficiency and reduced efficiency versus temperature for the segmented p-leg

Conclusions

This study took interest in the segmentation of thermoelectric materials. After recalling equations and significant quantities such as the compatibility factor or the maximum of reduced effciency, curves are plotted for several n-type and p-type thermoelectric materials. A particular attention was paid on the evolution of the reduced efficiency versus the relative current density. The investigation of these curves, rather than a 3D representation (that has already been plotted but not easy to interpret) allows to know if it is interesting or not to segment thermoelectric materials together. Then the example of a segmented leg with three p-type materials has been investigated with the use of the quantities previously cited.

Further developments will take interest in the whole efficiency of a thermoelectric generator device and especially focus on the influence of the hot or cold temperature on it.

Acknowledgments

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