Influence of the VO_2 metal-insulator transition on the thermoelectric properties of composites based on a $Bi_{0.5}Sb_{1.5}Te_3$ matrix

Alvarez-Guerrero S(1)*, Ordonez-Miranda J(2, 3), De Coss R(1), Alvarado-Gil JJ(1)

(1) Departamento de Física Aplicada, Centro de Investigación y de Estudios Avanzados del I.P.N-Unidad Mérida, Carretera Antigua a Progreso km. 6, A.P. 73 Cordemex, Mérida, Yucatán 97310, México.
(2) LIMMS, CNRS-IIS UMI 2820, The University of Tokyo, Tokyo 153-8505, Japan.
(3) Institute of Industrial Science, The University of Tokyo, Tokyo 153-8505, Japan.

*Corresponding author's email: santiago.alvarez@cinvestav.mx

Thermoelectric (TE) materials enable direct and reversible heat-into-electricity conversion, for constituting the basis for green and environment-friendly energy technology. Considerable effort has been devoted to improving the efficiency of BiTe-based materials. Currently, methods for improving the performance of TE materials are related to the use of low dimensionality for decreasing the phonon thermal conductivity and increasing the product S^2n, where S is the Seebeck coefficient and n is the charge carrier concentration. It is well known that thermoelectric properties of strongly correlated electron systems could contribute to the semiconductor to metal transition (SMT) [1]. Vanadium dioxide (VO_2) is a strongly correlated oxide [2], which shows a SMT close to room temperature, which induces remarkable changes in its structural, optical, and electrical properties. These characteristics have made vanadium dioxide the basis in the development of a great diversity of technological applications, such as temperature sensors [3], energy storage media [4], thermally-driven radiative diodes [5], among others. However, VO_2 has received little attention in the field of thermoelectricity [2] and scarce applications for VO_2 in thermoelectricity has recently emerged [6,7].

Inspired by the fact that vanadium dioxide shows a fully reversible first-order metal-to-insulator transition accompanied by a relatively little change in its thermal conductivity and an abrupt jump by nearly two orders of magnitude in its electrical conductivity on heating [8], we have investigated the influence of VO_2 on the electrical conductivity, thermal conductivity and Seebeck effect for $VO_2/Bi_{0.5}Sb_{1.5}Te_3$ composites. We combine the Bruggeman scheme [9], considered as one of the most accurate for high filler volume fractions and the accuracy of the finite element methods [10] to evaluate the thermal conductivity, electrical conductivity, and Seebeck coefficient for composites of three different vanadium dioxide concentrations.

The ETC values as a function of temperature are plotted in Fig. 1(a), the inset in the figure shows a good agreement with the experimental results reported by Back et al. [7] within the temperature range for T < 350 K. from these results we estimate the interface thermal resistance between $Bi_{0.5}Sb_{1.5}Te_3$ and VO_2 as R = 1.91 m^2KGW^{-1}. Figure 1(b) shows the dimensionless thermoelectric figure of merit (*ZT*) for pure $Bi_{0.5}Sb_{1.5}Te_3$ and for the composites as function of temperature. It can be observed that *ZT* values of all composites increase with increasing temperature to reach a maximum value and then to decrease with further increase in temperature. Moreover, the *ZT* values significantly increased with the incorporation of VO_2 nanoparticles and it is notable that there is a good agreement between the experimentally determined *ZT* values and our calculations of $VO_2/Bi_{0.5}Sb_{1.5}Te_3$ composites for f = 29.4% VO_2. The low *ZT* values of composites at low temperatures is a consequence of changes that

VO_2 undergoes for both thermal and electrical properties. Nevertheless, the composite with f = 34.0% exhibited a maximum ZT value of ~0.7 at 375 K, which is around 10% higher than that of BST matrix. For higher temperatures, the figure of merit values showed a significant improvement of around 20% compared with pure $Bi_{0.5}Sb_{1.5}Te_3$. Thus, this improvement is primarily due to the enhancement of the electrical conductivity and reduction in thermal conductivity.

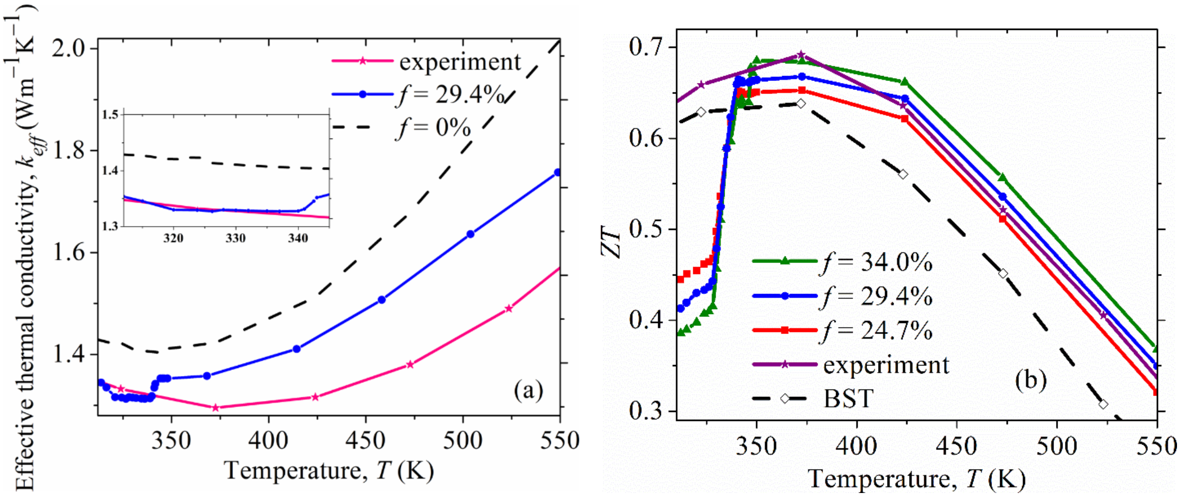

Fig. 1. (a) Comparison between the temperature dependence of the thermal conductivity of the experimental results and our simulations. **(b)** Comparison between the ZT calculated values and the experiment [7]

Conclusions – The thermoelectric properties of $VO_2/Bi_{0.5}Sb_{1.5}Te_3$ composites with volume fractions of 0, 24.7%, 29.4% and 34.0% have been investigated across the metal-insulator transition of VO_2 and for temperatures up to 550 K, by means of simulations based on Finite Element Methods. We have shown that VO_2 nanoparticles with a concentration of 34.0% enhance the electrical conductivity by approximately 16% for temperatures higher than 350 K. The resulting maximum value of ZT = 0.7 shows up at 375 K, which represents an increase of 10% in comparison with the corresponding one of the matrix.

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