複数の空間電荷モデルによる熱電特性の解析

Thermoelectric property analyzed by space charge models

株式会社テクノプロ, テクノプロ R&D 社 ○掛本 博文 [1]
[1]Techno Pro R&D company, Techno Pro Inc., ○Hirofumi Kakemoto[1]

1. Introduction

Recently, large thermal electromotive force (EMF) and Seebeck coefficient (S) are reported in experimental studies about oxide TE materials [1,2] and their values can be partly estimated by space charge model. Thermoelectric (TE) properties of various TE materials are possible to be understood by Fermi integral method, narrow band model [3], and space charge model.[4] The space charge (SC) model is proposed by Mahan. SC model is defined at low temperature. [Mahan] In addition to above theory, large EMF is possible to generate from interface between electrode and sample. Here, we tried to modify the SC model with defect structure [5] and interface of electrodes in order to estimate TE properties in high temperature, and their results are reported.

2. Calculation

Thermal electromotive force (EMF) generated from the contact between TE material and electrodes (short length EMF). Thermoelectric (TE) properties were calculated combined with interface around electrodes and inner space charge effect, as shown in **Fig 1**.

2-1 Interface charge effect

Inner thermal EMF carrier charging around electrode was simply calculated from current density due to inner electric field, as shown in **Fig.1(a)**, $(4/3)V_{ele}^{3/4}=2(-J/\varepsilon\varepsilon_o)^{1/2}(m^*/2e)^{1/4}x+2SdT$, where carrier charging effect on electrode (first term), and usual thermal EMF (second term), as follows $V_o=2V_{ele}+2SdT$, (1)

where _, _, and _ are _, _, and _, respectively. [6]

2-2 Inner space charge effect

Thermal EMF by SC was also calculated by using Poisson's eq. ($d^2V(x)/dx^2= -e\delta n(x)/\varepsilon$), as shown in **Fig.1(b)**. Thermal EMF and S are estimated, as follows,

$V_1=|V(L)/V(0)|=(\varepsilon/q_D)[q_DL(1+\exp(-q_DL)+2\exp(-q_DL)-2]$, (2)

$S=-(V/dT)\{f(q_DL)\}$, (3)

where $f(q_DL)=1-(2/q_DL)\tanh(q_DL/2)$, and n, q_D, L, and ε are __, __, __, and __, respectively. [4, 5]

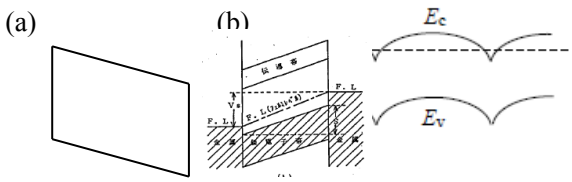

Fig. 1 Band diagrams, (a) interface charge at electrodes and inner electric field (n-type), and (b) space charge and defect structure.

3. Results

Figure 2 shows thermal EMF profile as a function of x. High values are estimated at around interfaces between semiconductor and electrodes.

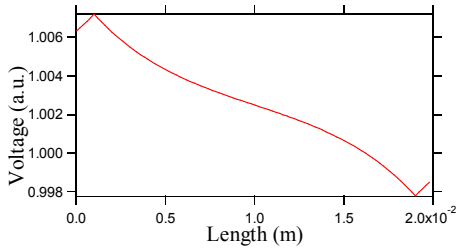

Fig. 2 EMF: V profile as a function of x. (parameters: ε_r, dT=10K, 温度)…

The voltage distribution of interface (x=0, 20mm) and inner sample is observed as a function of length (x), as shown in **Fig.1**. The EMF is increased by charging effect around both interfaces, in addition to space charge effect.

4. Conclusion

Thermoelectric properties were calculated for (1) carrier charging around electrode, and (2) space charge (SC) in inner TE material. The carriers are thermally diffused for electrode accompanied with inner SC, and thermal EMF from (1) carrier charging is effective for large S in addition to (2) inner SC effect, and it is origin of huge EMF.

In future study, reducing instability for polarity, caused by huge EMF in the area of interface will be investigated. (Need more examples.)

References

[1] Ohta and Koumoto et al., Nat. Mat, **6**, 129-134, (2007).
[2] Zhang and Ohta et al., Nat. Commun. **9**, 2224 (2018).
[3] H.Kakemoto, ACS Applied Electronic Materials (Letter), **1**, pp.2476-2482, (2019).
[4] Mahan, J. Electronic Materials, **44**, 431, (2015). (phonon drag ではない)
[5] H.Kakemoto, The 65th JSAP Spring Meeting 2018, 18a-P3-13.誘電率を増大
[6] Thermal EMF carrier charging calculated from current density due to inner electric field.
$J=Nev$, $v=(2eV/m^*)^{1/2}$, $\rho=-Ne=J/v=-J(2eV/m^*)^{-1/2}$
$d^2V/dx^2=\rho/\varepsilon\varepsilon_o=-(J/\varepsilon\varepsilon_o)(m^*/2eV)^{1/2}$
$(dV/dx)^2=-4JV^{1/2}/(\varepsilon\varepsilon_o(2e/m^*))+C_1$
$(4/3)V^{3/4}=2(-J/\varepsilon\varepsilon_o)^{1/2}(m^*/2e)^{1/4}x+C_2$
$V_o=V_{o1}+SdT$, where SdT is caused EMF from dT.
[7] H.Kakemoto, to be submitted.