空間電荷モデルによる熱電特性

Thermoelectric properties calculated by space charge model

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1. Introduction

Thermoelectric (TE) properties of various TE materials are possible to be understood by Fermi integral method [1], narrow band model [2,3], and space charge model [4]. Seebeck coefficient (S) of TE material is usually measured within Somerfeld approximation: $S \sim T$. In Recent, however, high S values (200μV/K) are reported in experimental studies about oxide TE materials, and their values can be estimated by space charge model.

The space charge model is proposed by Mahan [4], and is defined at low temperature. Here, we tried to modify the space charge model with defect structure [5] in order to estimate TE properties in high temperature, and its results are reported.

2. Calculation

Thermoelectric (TE) properties was calculated by using space charge model.[4] Figure 1 shows space charge model in this study.[5] Thermal electromotive force (EMF) is obtained by using Poisson's eq. ($d^2V(x)/dx^2 = -e\delta n(x)/\varepsilon$), as follows,

$$|V(x)-V(0)| = (\varepsilon/q_D)[xq_D(1+\exp(-q_DL) + \exp(-q_DL)+\exp(-q_Dx)-1-\exp(-q_D(L-x))] \quad (1),$$

where q_D, n, and ε are Debye length, carrier density, and dielectric permittivity ($\varepsilon_r\varepsilon_0$), respectively.

Total EMF and Seebeck coefficient (S) are estimated, as follows,

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

$$S = -V/dTf(q_DL) \quad (3),$$

where $f(q_DL) = 1-(2/q_DL)\tanh(q_DL/2)$.

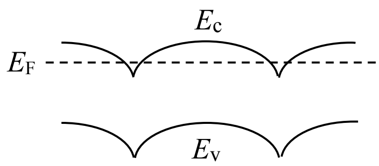

FIG.1 Defect structure model in this study.

3. Results and discussion

Figure 2 shows the total EMF calculated by eq.(2), and temperature dependence of Seebeck coefficient (S) calculated by using eq.(3). In calculation, the effective defect in Fig.1 was considered as the origin of space charge.

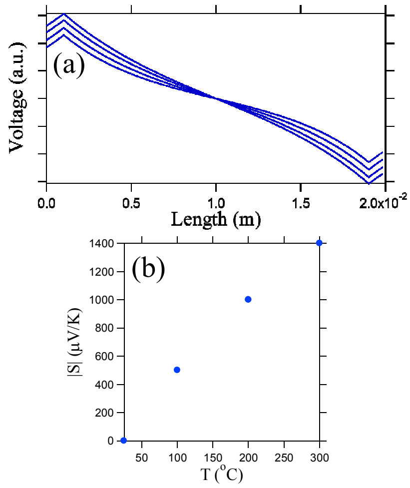

FIG.2 (a) EMF profiles calculated by space charge model, (b) TE properties calculated by using eq. (2,3).

4. Conclusion

Thermoelectric (TE) property of TE material was calculated by space charge model. (1) As the origin of space charge, for example, effective defect at grain and grain boundary of TE material was considered, and space charge distribution was defined by Poisson's equation.

(2) Thermal electromotive force (EMF) and Seebeck coefficient (S) were calculated with Debye length, carrier density defined by Poisson's equation, and dielectric permittivity. Temperature dependence of TE property: for example, S for oxide TE material was calculated.

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Reference

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