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Numerical Analysis of the Boundary Scattering Effect on Transport Properties in Bi-Sb Nanowires

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In this study, we have numerically analyzed the transport properties of Bi-Sb nanowires, taking into account wire boundary scattering. Wire boundary scattering slightly decreased the Seebeck coefficient of Bi-Sb nanowires. This effect is due to the observation that boundary scattering and the mobility ratio of L-point electrons to T-point holes in the nanowires are smaller than those in bulk Bi-Sb because the wire boundary scattering suppresses the mobilities of L-point electrons and heavy holes. The largest Seebeck coefficient for all wire diameters was obtained when the Sb concentration was 5 at.%. The effective mass approached zero near 5 at.% Sb, and the small effective mass led to a large subband shift in each band. Thus, a small effective mass enhances the quantum effect at a fixed wire diameter, even if wire boundary scattering is taken into account.

Key words: Transport properties, Bi-Sb, nanowire, wire boundary scattering

INTRODUCTION

Thermoelectric efficiency is characterized by the thermoelectric figure of merit, $Z = \alpha^2\sigma/\kappa$, where α, σ, and κ represent the Seebeck coefficient, electric conductivity, and thermal conductivity, respectively. A theoretical suggestion on how to improve the thermoelectric efficiency of Bi nanowires has been reported.[1] Bismuth, as a semimetal, has interesting electrical properties such as small effective mass, low carrier density, and long mean free path, and the properties of bismuth, such as its Fermi surface and effective mass, have been well studied.[2,3] The small effective mass easily produces the quantum effect in nanowires. Moreover, the quantum effect enhances the Seebeck coefficient, and the thermoelectric performance can be improved. It is well known that addition of Sb to bulk Bi changes the Bi band structure, leading to a significantly small effective mass.[4] Addition of Sb to Bi nanowires can also improve their thermoelectric properties.[5] However, estimated transport properties of such nanowires reported in previous literature used bulk mobility values without including the effects of wire boundary scattering. Recently, Murata et al. reported that wire boundary scattering changes the transport properties in Bi nanowires.[6] In this study, we numerically analyzed the transport properties of Bi-Sb nanowires, taking account of wire boundary scattering.

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CALCULATION MODEL

The electronic structure in Bi-Sb nanowires was analyzed by numerically solving the effective mass equations for electrons and holes.[1] It was assumed that the carriers are confined within the nanowire. The effective mass equations at the T- and L- points are

$$-\frac{\hbar^2}{2}\nabla\cdot M_{\mathrm{T}}^{-1}\cdot\nabla\Psi(r) = E\Psi(r), \tag{1}$$

$$M_{\mathrm{T}} = \begin{pmatrix} m_{\mathrm{T1}}^* & 0 & 0 \\ 0 & m_{\mathrm{T2}}^* & 0 \\ 0 & 0 & m_{\mathrm{T3}}^* \end{pmatrix}, \tag{2}$$