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Grain-Size-Dependent Thermoelectric Properties of $SrTiO_3$ 3D Superlattice Ceramics

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The thermoelectric (TE) performance of $SrTiO_3$ (STO) 3D superlattice ceramics with 2D electron gas grain boundaries (GBs) was theoretically investigated. The grain size dependence of the power factor, lattice thermal conductivity, and ZT value were calculated by using Boltzmann transport equations. It was found that nanostructured STO ceramics with smaller grain size have larger ZT value. This is because the quantum confinement effect, energy filtering effect, and interfacial phonon scattering at GBs all become stronger with decreasing grain size, resulting in higher power factor and lower lattice thermal conductivity. These findings will aid the design of nanostructured oxide ceramics with high TE performance.

Key words: Thermoelectrics, perovskite oxides, Boltzmann transport equation, energy filtering effect

INTRODUCTION

Oxide ceramics with nanometer grain size are promising high-performance, environmentally benign thermoelectric (TE) materials.[1] Their TE performance depends on the dimensionless figure of merit, $ZT = S^2\sigma T/\kappa$, where S, σ, κ, and T are the Seebeck coefficient, electrical conductivity, thermal conductivity, and absolute temperature, respectively. In order to enhance the ZT value of nanostructured ceramics, grain boundaries (GBs) have been widely used as functional interfaces to reduce the lattice thermal conductivity[2] or to enhance the power factor.[3] Using nanostructured ceramics to reduce the lattice thermal conductivity has been reported in many material systems,[4] and in some systems even the minimum value was approached.[5] There are also several studies regarding the realization of the energy filtering effect by the GB potential barrier to enhance the power factor, both theoretically[6] and experimentally.[7] However, there are few reports about the influence of the quantum confinement effect on the TE properties of nanostructured ceramics.

In our previous work, realization of the quantum confinement effect at GBs and its influence on the TE performance of nanostructured ceramics were investigated theoretically.[8] Quantum confinement occurs when the dimension of the system is comparable to the electronic wavelength; the electronic structure and hence the transport properties are different from in the bulk.[9] It was reported that the quantum confinement effect due to a 2D electron gas (2DEG) greatly enhances the TE performance in $SrTiO_3$/Nb:$SrTiO_3$ superlattices.[10,11] In our previous theoretically simulations,[8] the 2DEG formed at GBs, which gives rise to the quantum confinement effect, also enhances the power factor and ZT value of the nanostructured ceramics, and the ceramic with grain size of 6.4 nm exhibited $ZT = 1.13$ at room temperature. However, it is very hard to obtain ceramics with such small grain size.[2] So, the TE performance of ceramics as a function of grain size should be evaluated to understand the grain size effect on TE performance. In this work, using our improved simulation methods (compared with our previous work), the grain size dependence of

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