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Thermoelectric Properties of Polycrystalline Bilayer Graphene under Vertical Electric Field

Thermoelectric (TE) generation is a potential key technology for recovering energy from waste heat. Among the various potential candidates for TE materials, nanocarbon materials have attracted attention as flexible and high-performance TE materials. Most recently, Yamamoto and Fukuyama reported that the semiconducting carbon nanotubes (CNTs) exhibit high TE performance when the chemical potential μ locates near a band edge with a sharp density of states (DOS) originating from its one dimensionality [1,2]. On the other hand, the graphene, which is a two-dimensional honeycomb lattice consisting of carbon atoms, cannot be expected to be high-TE performance because it has no band gap at the charge neutral point. In this study, we focus on the bilayer graphene (BLG) since the band gap of BLG can be opened by applying the vertical electric field [3] in contrast to the ε-linear DOS of monolayer graphene as shown in Fig. 1. We have calculated the Seebeck coefficient S and the power factor PF of the BLG in the presence of vertical electric field $E_\perp$ using the Kubo's linear response theory combined with thermal Green's function method which was recently developed [1,2]. We adopt the constant-τ approximation for self-energy due to carrier scattering [2]. We found that the values of S and PF can be controlled by changing the magnitude of $E_\perp$. For example, we obtained $S \sim 200$ μV/K and $PF \sim 40$ mW/mK^2 when μ lies close to a band edge and the vertical electric field is $E_\perp = 4.8$ MV/cm. This is because the DOS of BLG under $E_\perp$ has a sharp peak near the band edge, which is similar to carbon nanotubes. Next, to confirm the validity of our theoretical results of TE effects of BLG, we compared with the TE measurements of a polycrystalline BLG by using electronic double layer gating technique [4]. As a result, the theoretical results are in excellent agreements with the experimental data when $\tau \sim 10$ fs. Under the assumption that τ is determined by the grain boundary scattering of the polycrystalline BLG, the averaged grain diameter d_{grain} can be calculated as $d_{\mathrm{grain}} \approx 10$ nm, which is comparable to the typical grain diameter of the polycrystalline BLG sample estimated from the Raman spectroscopy [5]. Furthermore, we investigated effects of the crystallinity of polycrystalline BLGs on their TE properties. The maximum value of S monotonically increases with increasing d_{grain} and it is saturated at $d_{\mathrm{grain}} \sim 100$ nm. This means that the crystalline with $d_{\mathrm{grain}} > 100$ nm is needed to maximize the Seebeck coefficient of BLG.

References

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Figures

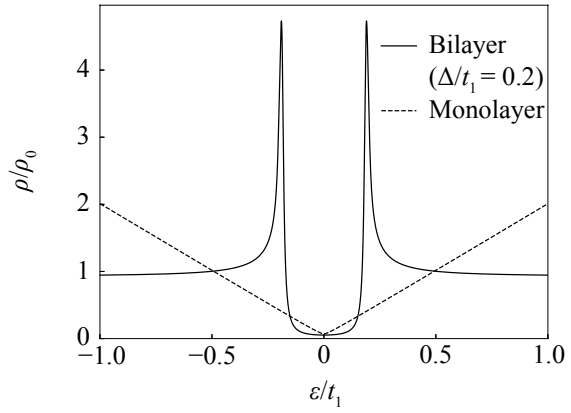

Figure 1: Density of states (DOS) of bilayer graphene (BLG) under vertical electric field and monolayer graphene. Here, Δ is a half value of potential difference between layers caused by vertical electric field, t_1 is inter-layer hopping integral in BLG, and ρ_0 is DOS of BLG for Δ = 0.