Enhancement of thermoelectric properties in in-plane Graphene/BN structures

Van-Truong Tran, Jérôme Saint Martin, Philippe Dollfus
IEF, Université Paris-sud, CNRS, UMR 8622, Bât 220, 91405 Orsay, France.
Emails: van-truong.tran@u-psud.fr and philippe.dollfus@u-psud.fr

Abstract

In spite of the remarkable advantage of excellent electron transport properties [1,2], graphene has two major drawbacks with a view to thermoelectric applications. First, this material is a gapless semimetal, which makes difficult to separate the opposite contributions of electrons and holes to the Seebeck coefficient. Second, it exhibits very high lattice thermal conductivity [3]. Different strategies of nanostructuring have been suggested to open a bandgap, enhance the Seebeck coefficient and reduce the thermal conductivity of graphene, and finally to achieve good values of thermoelectric figure of merit *ZT* (see review [4]). In the simple case of a graphene ribbon, the highest *ZT* value achievable at room temperature is about 0.35 for a very narrow armchair ribbon with 3 dimer lines (M_{CC} = 3) along the width.

Here, taking advantage of the fact that recently a novel form of a hybrid monolayer material of graphene and Boron Nitride has been synthesized successfully [5,6], we propose a new structure of graphene/BN, as schematized in Fig 1, expected to enhance thermoelectric performance. By means of atomistic simulation of electron and phonon transport, we show that the phonon conductance is strongly reduced in this structure because of high scattering at the edges and at graphene/BN interfaces. Additionally, a good power factor is achieved thanks to the bandgap opening in the graphene/BN regions. These combined results lead to a significant enhancement of *ZT*. In Fig 2, we plot *ZT* as a function of chemical potential for a structure of graphene width M_{CC} = 5. A peak *ZT* as high as 0.81 at room temperature is obtained for a chemical energy μ = 0.41 eV, and *ZT* = 1.48 is even reached if three vacancies are introduced in the channel (not shown). It is remarkable that such high value can be obtained at relatively low and quite accessible chemical energy.

References

[1] P.J. Zomer, S.P. Dash, N. Tombros and B.J. Van Wees, Appl. Phys. Lett. 99 (2011) 232104.
[2] A.H. Castro Neto, N.M.R. Peres, K.S. Novoselov, and a. K. Geim, Rev. Mod. Phys. **81** (2009) 109.
[3] A.A. Balandin, S. Ghosh, W. Bao, I. Calizo, D. Teweldebrhan, F. Miao and C.N. Lau, Nano Lett. 8 (2008) 902-907.
[4] P. Dollfus, V. Hung Nguyen, J. Saint-Martin, J. Phys.: Condens. Matter 27 (2015) 133204.
[5] P. Sutter, R. Cortes, J. Lahiri and E. Sutter, Nano Lett. 12 (2012) 4869–4874.
[6] Z. Liu, L. Ma, G. Shi, W. Zhou, Y. Gong, S. Lei, X. Yang, J. Zhang, J. Yu, K.P. Hackenberg, A. Babakhani, J.-C. Idrobo, R. Vajtai, J. Lou and P.M. Ajayan, Nat. Nanotechnol. 8 (2013) 119-124.

Figures

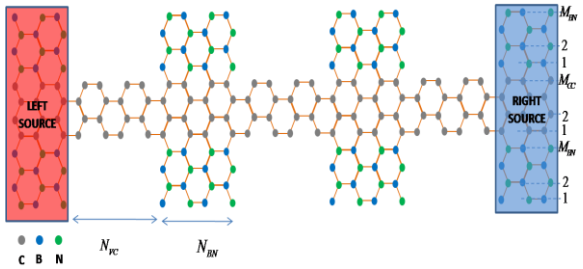

Fig 1: Studied structure with BN flakes attached to a graphene ribbon in the channel. We define n_{BN} as the number of BN/G/BN sections in the active region.

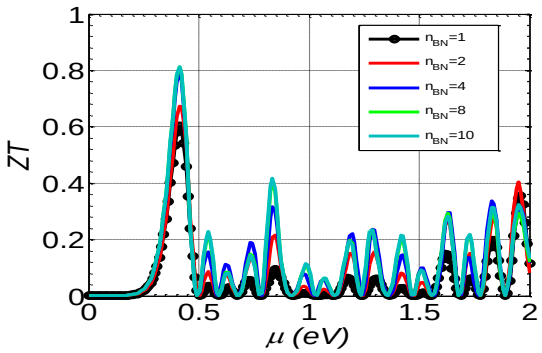

Fig 2: Figure of merit *ZT* as a function of chemical potential for different values of n_{BN}. The structure parameters are M_{CC} = 5, M_{BN} = 9, N_{VC} = N_{BN} = 8. Simulation was performed at *T* = 300 K.