Journal Name

ARTICLE TYPE

Cite this: DOI: 10.1039/xxxxxxxxxx

Supplementary Material of Thermal and electronic transport characteristics of highly stretchable graphene kirigami†

Bohayra Mortazavi,[a‡] Aurélien Lherbier,[b‡] Zheyong Fan,[c,d‡] Ari Harju,[d] Timon Rabczuk,[e] and Jean-Christophe Charlier[b]

Received Date
Accepted Date

DOI: 10.1039/xxxxxxxxxx

www.rsc.org/journalname

1 Electronic diffusivity

In order to display the complex dynamics of charge carriers taking place in the kirigami structures one discusses here the directional, energy and time dependent diffusivities. The diffusivities along the x direction ($D_x(E,t)$) and along the y direction ($D_y(E,t)$) are presented in Fig.1 for five selected energies E =-0.4, -0.2, 0.0, +0.2, and +0.4 eV with respect to the Fermi energy (E_F). The top panels of Fig.1 correspond to θ_c=0°, the middle panels to θ_c=90°, and the bottom panels to θ_c=180°. First, one notices that $D_y(E,t)$ is systematically lower than $D_x(E,t)$ by one or two orders of magnitude, indicating a clear anisotropy in the two transport directions. Second, the magnitude of the diffusivity is dependent on the energy which can be understood from the complex DOS containing numerous van Hove singularities and possible band gaps as observed in main text in Fig.**??**. Some diffusivity curves exhibit significant undulations which can introduced by the numerical derivatives of wave packet quadratic spreading ($\frac{\partial \Delta X^2(E,t)}{\partial t}$, $\frac{\partial \Delta Y^2(E,t)}{\partial t}$), in particular for long cut lengths l_c =80 and 160 nm. In some cases, it even induces a negative value of the diffusivity because in the localization regime the saturating quadratic spreading is no more increasing monotonically and may slightly oscillate, i.e. has a small negative slope. This is a possible artifact of the calculation. One also observes that the long time ballistic regime discussed in the main text in section **??** is easily observed for l_c =10 nm (red curves) but is not clearly obtained for the other systems. For (θ_c,l_c)=(0°,20 nm), the diffusivities are found to be anomalously low compared to other systems. However, this can be rationalized by the fact that a rather large band gap with localized states were observed in the vicinity of the Fermi level for this (θ_c,l_c)=(0°,20 nm) graphene kirigami. Some diffusivity curves display a diffusive regime i.e. a constant value of $D(t)$ (see for instance $D_x(E,t)$ and $D_y(E,t)$ of the (θ_c,l_c)=(180°,160 nm) for E=-0.4, +0.2 and +0.4 eV), which results from the scattering at the cut edges. In other cases, a localized regime is observed i.e. a zero value of $D(t)$ corresponding to constructive quantum interferences in scattering loops inducing localization of the wave packet. However, as mentioned in main text in section **??**, at longer propagation time the diffusivity should finally recover a ballistic behavior because of the periodicity. Overall, Fig.1 demonstrates the complex transient regimes that can be obtained in these graphene kirigami structures.

[a] *Institute of Structural Mechanics, Bauhaus-Universität Weimar, Marienstr. 15, D-99423 Weimar, Germany; E-mail: bohayra.mortazavi@gmail.com*
[b] *Université catholique de Louvain, Institute of Condensed Matter and Nanosciences, Chemin des étoiles 8, 1348 Louvain-la-Neuve, Belgium; E-mail: aurelien.lherbier@uclouvain.be*
[c] *School of Mathematics and Physics, Bohai University, Jinzhou, China*
[d] *COMP Centre of Excellence, Department of Applied Physics, Aalto University, Helsinki, Finland; E-mail: zheyong.fan@aalto.fi*
[e] *College of Civil Engineering, Department of Geotechnical Engineering, Tongji University, Shanghai, China*
† Electronic Supplementary Information (ESI) available: [See SupMat.tex SupMat.pdf]. See DOI: 10.1039/b000000x/
‡ These authors contributed equally to this work

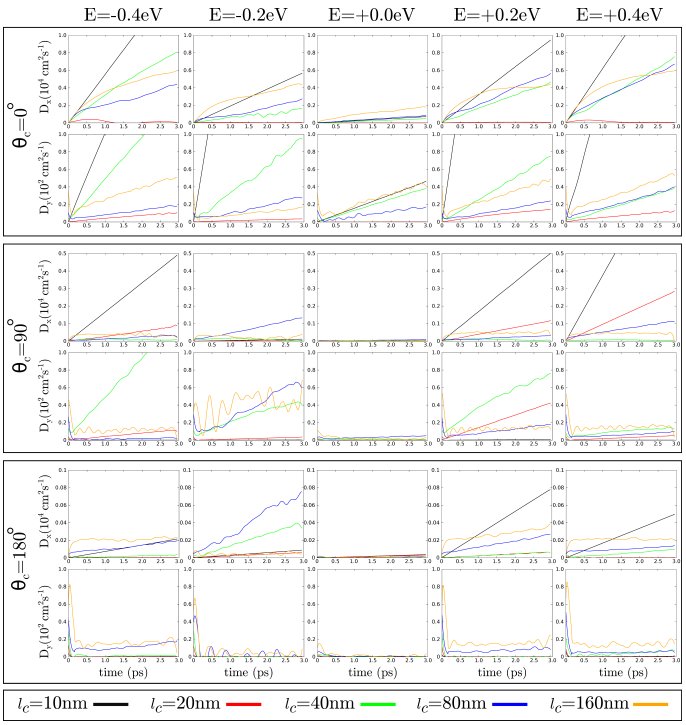

Fig. 1 Energy and time dependent diffusivity ($D_x(E,t)$ and $D_y(E,t)$) for different kirigami structures with cut angles θ_c=0, 90, and 180°, cut lengths l_c=10, 20, 40, 80, and 160 nm.

2 Heat Flux profiles

To better explain the reason why graphene kirigami structures present highly anisotropic thermal conductivity, i.e. a much higher thermal conductivity along the transverse direction than the longitudinal one, we present in Fig.2 samples of heat flux profiles obtained using the finite element method. For the longitudinal heat transfer, the cuts directly obstacle the heat transfer and as a result some parts of the material do not involve in the heat transfer. On the other side, for the heat transfer along the transverse direction, the cuts are parallel to the heat flow and in this case the material are very uniformly involved in the heat flux transfer.

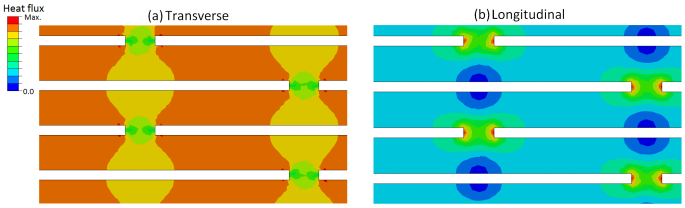

Fig. 2 Sample of heat flux profiles computed using the finite element method for the thermal transport along the transverse and longitudinal directions.