Flowered graphene: Growth, charge and thermal transport

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Flower defects are the smallest dislocation loops observable in graphene. In this contribution [1], we illustrate their structural and transport properties investigated by means of high-resolution transmission electron microscopy and multiscale simulation tools based on density functional theory, Green's functions and Boltzmann transport equation. On the basis of our experimental images, we propose that flower defects are the grains *left over* by a bulge-type mechanism during the dynamic recrystallization of CVD graphene [2]. In order to explore their properties and the potential applications, we simulate electron and phonon transport in large graphene samples with different densities of flowers. At large densities, an energy-filtering effect is observed, with an almost unaffected hole transport and a significantly suppressed electron transport. This asymmetry originates from the flower-broken sublattice symmetry. For the same flower densities, heat transport is strongly decreased as a consequence of the dominant elastic scattering induced by the defects. Interestingly, even for low flower concentrations, the contribution of flexural phonons, which is significant in pristine graphene, is largely suppressed.

References

[1] A. Cresti *et al.*, Carbon, 161 (2020) 256
[2] A. Tyurnina *et al.*, Carbon 102 (2016) 499

Figures

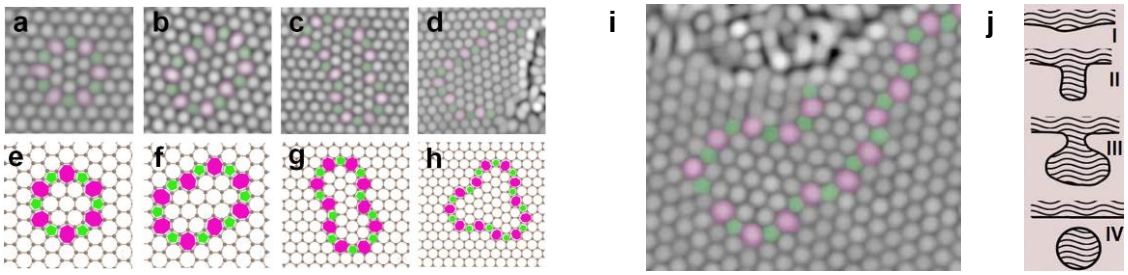

Figure 1: (a-d) Experimental and (e-h) DFT-calculated flower-related defects. (i) Bulge corresponding to stage II or III in the nucleation mechanism sketched in (j).

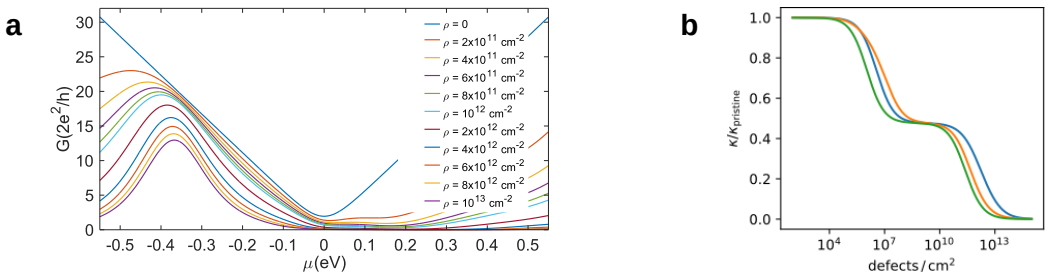

Figure 2: (a) Room-temperature conductance vs chemical potential of a 50 nm-wide graphene ribbon with different flower (fig.1a) densities. (b) Room-temperature thermal conductivity of graphene with varying concentration of T_0 Stone-Wales, T_1 flower (fig.1a) and T_2 flower (fig.1h) defects.