Spin transport in polycrystalline graphene

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Owing to its small spin-orbit coupling (SOC) and high electron mobility, graphene has proven to be an efficient transporter of spin, making it a promising material for spintronics [1]. Meanwhile, chemical vapor deposition (CVD) is the best route for producing industrial-scale graphene [2]. Graphene grown by CVD tends to be polycrystalline, with disordered grain boundaries (GBs) separating misoriented grains [3]. While preliminary experiments have been done [4], so far little theoretical work has explored the detailed nature of spin transport in realistic models of CVD-grown graphene.

Here we present our recent work along these lines. We first use *ab initio* simulations to derive a tight-binding model which accounts for modified SOC parameters introduced by GBs. We then apply these models to real-space wave packet simulations [5] that allow us to study spin transport in large-area polycrystalline graphene samples (Fig. 1).

We find that the spin lifetime scales inversely with the graphene grain size, as expected from typical D'yakonov-Perel' (DP) theory. However, this theory also significantly underestimates the calculated spin lifetimes (Fig. 2). In order to explain this discrepancy, we update the DP theory to account for quantum interference and localization effects, which are naturally present in polycrystalline graphene and alter the conventional theoretical framework developed in the semiclassical diffusive regime.

References

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[2] Zhang et al., Accounts Chem. Res. 46 (2013) 2329-39
[3] Isacsson et al., 2D Mater. 4 (2017) 012002
[4] Kamalakar et al., Nat. Commun. 6 (2015) 6766
[5] Fan et al., arXiv:1811.07387 (accepted to Rev. Mod. Phys.)

Figures

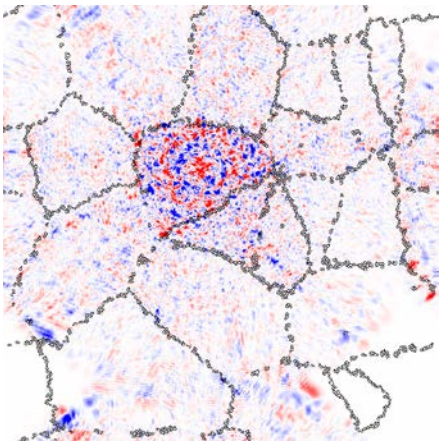

Figure 1: Simulation of spin-dependent wave propagation in polycrystalline graphene.

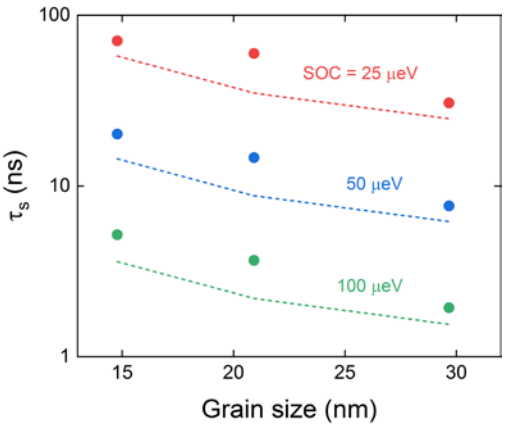

Figure 2: Spin lifetime as a function of graphene grain size. Symbols are numerical results, and dashed lines are from semiclassical DP theory.