Electronic transport in doped polycrystalline graphene

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Abstract

Graphene as a raw material for electronic devices is frequently synthetized using chemical vapor deposition (CVD), which is a reliable way to get a large area graphene sample [1]. Usually, CVD graphene consists of a variety of misoriented graphene grains with grain boundary interfaces. These grain boundaries are made up of non-hexagonal carbon rings which degrade the electrical and mechanical properties. Also, these interfaces have a high chemical reactivity that suggests a promising chemical detection mechanism that is not fully understood so far.

We present numerical simulations of quantum transport in functionalized polycrystalline graphene samples using tight binding parameters extracted from the literature for hydrogen and epoxide groups [2, 3]. To carry out the transport calculations we use a real-space order-N quantum wave packet approach to compute the Kubo-Greenwood formula, which we then relate to the mobility as a function of carrier concentration in order to match with experimental measurements [4, 5]. In order to understand the effect of the dopants on the CVD graphene we set up two different situations: a random doping distribution and an accumulation of the doping at the grain boundaries. Our calculations support experimental measurements that reveal distinct electronic transport regimes depending on the density and distribution of induced defects on the polycrystalline graphene films (Figure 1, [5]). Our findings provide a novel perspective to tailor the properties of polycrystalline graphene

References

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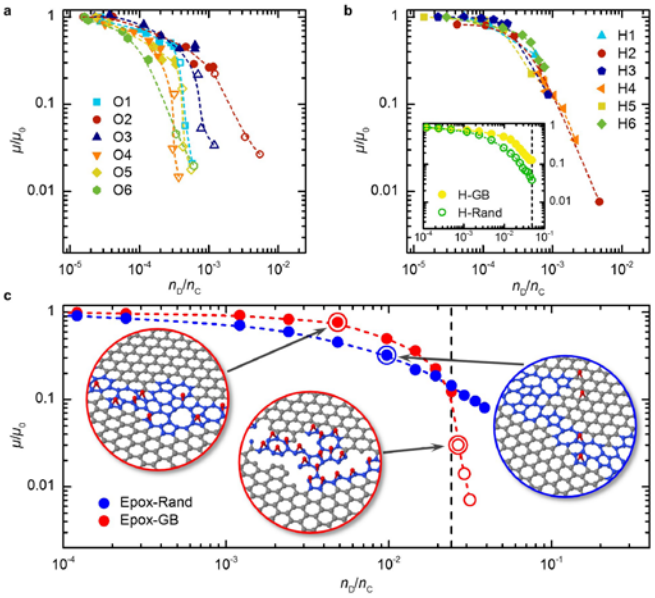

Figure 1. Electronic transport in functionalized CVD graphene. a and **b**, Field-effect mobility as a function of the relative defect density for six different transistors (each symbol representing a device) for graphene oxidation and hydrogenation, respectively. The mobility data are normalized to the mobility of clean devices. Open symbols represent ozone treatments at substrate temperatures above 70°C. The relative defect density n_D/n_C was calculated from the integrated area D/G Raman intensity ratio; nine measurement spots within the 10x10 μm^2 transistor channels were averaged to create one data point. **b** (inset)**,** Simulation of μ/μ_0 for increasing amount of hydrogen defects with a random distribution (green) and accumulated at grain boundaries (yellow). The vertical dashed line represents the saturation of the grain boundaries with hydrogen. **c**, Simulation of μ/μ_0 for an increasing amount of epoxide defects with random distribution (blue) and accumulated at grain boundaries (red). After reaching the saturation threshold of the grain boundaries by epoxide defects (vertical dashed line), vacancies are gradually added (open symbol data points).