Grain boundary-induced variability of charge transport in hydrogenated polycrystalline graphene - DTU Orbit (10/01/2019)

**Grain boundary-induced variability of charge transport in hydrogenated polycrystalline graphene**

Chemical functionalization has proven to be a promising means of tailoring the unique properties of graphene. For example, hydrogenation can yield a variety of interesting effects, including a metal-insulator transition or the formation of localized magnetic moments. Meanwhile, graphene grown by chemical vapor deposition is the most suitable for large-scale production, but the resulting material tends to be polycrystalline. Up to now there has been relatively little focus on how chemical functionalization, and hydrogenation in particular, impacts the properties of polycrystalline graphene. In this work, we use numerical simulations to study the electrical properties of hydrogenated polycrystalline graphene. We find a strong correlation between the spatial distribution of the hydrogen adsorbates and the charge transport properties. Charge transport is weakly sensitive to hydrogenation when adsorbates are confined to the grain boundaries, while a uniform distribution of hydrogen degrades the electronic mobility. This difference stems from the formation of the hydrogen-induced resonant impurity states, which are inhibited when the honeycomb symmetry is locally broken by the grain boundaries. These findings suggest a tunability of electrical transport of polycrystalline graphene through selective hydrogen functionalization, and also have implications for hydrogen-induced magnetization and spin lifetime of this material.

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