Realistic atomic-scale model for polycrystalline graphene and the related mechanical and electronic properties

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Large-scale production of graphene relies on chemical vapor deposition (CVD), which unfortunately leads to samples which have properties that are markedly different from those of mechanically exfoliated mono-layers. One reason for this is that CVD-growth initiates spontaneously on several different locations and often with random lattice orientations. When the separately grown grains meet, the structure gets patched with grain boundaries (GB) which consist of non-hexagonal carbon rings to make up for the mismatch in lattice orientations.

Although experimental studies have recently brought light onto the atomic structure of grain boundaries as well as their effect on the magnitude of changes in properties due to their influence, detailed atomic-scale understanding of the origin of the different properties has remained unknown. For this reason, we have established a method to create realistic atomistic models of polycrystalline graphene structures which have random misorientation angles between the different grains and exhibit serpent-like meandering GB structures similar to the experimental images. Using this model, we have shown that—unlike has often been expected—mechanical failure upon stretching a graphene sheet does not start from within individual GBs but rather at points where several GBs meet. From there, the cracks them propagate through the grains (not along the GBs), again similar to recent experimental findings. Our atomistic models have further allowed us to study the charge transport characte ristics in realistic polycrystalline graphene samples. Our calculations revealed a remarkably simple scaling law which relates several of the transport properties to the average grain sizes in the sample, establishing quantitative foundations for estimating transport features in polycrystalline graphene.