Vacancy mediated plastic deformation in graphene

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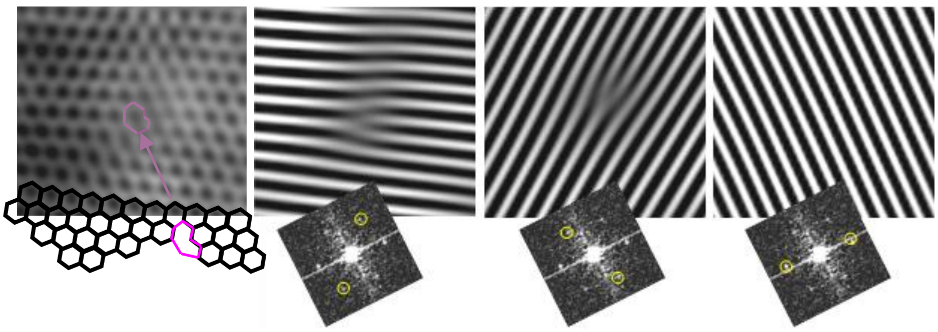
Plasticity and ductile failure in graphene and carbon nanotubes can be mediated through dislocation glide by "Stone Wales" type bond rotations. While the reaction barrier for such bond rearrangements is high, they can be catalysed, for example through the presence of an interstitial carbon atom. We show here that vacancies can act as sources for shuffle dislocations, whose migration barrier is typically four times lower than that of classical glide edge dislocations.

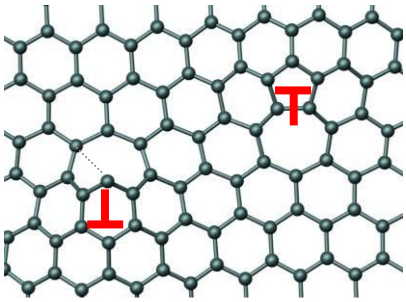
We confirm the existence and structure of shuffle--glide dislocation pairs in graphene via high resolution electron microscopy, supported by density functional calculations.

Vacancies and other dislocation cores can also act as sinks for migrating dislocations. This leads to a new model for ductility and super-plasticity in carbon nanotubes, for example under irradiation, where vacancies emit and absorb rapidly migrating shuffle dislocations. The model is consistent with recent experimental observations of superplasticity in electron irradiated nanotubes under tensile strain. The dislocation pairs induce buckling in the basal plane of the graphene and may represent a very common intrinsic defect species.

Figures



Shuffle dislocation core in graphene viewed using HAADF, with image filtering applied (image construction using only specific points from the electron diffraction).



Possible separation of a mono-vacancy into a pair of dislocations (one glide, one shuffle) via motion of the shuffle dislocation core.