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Atomic-scale investigation of grain boundary motion in graphene

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Grain boundaries (GBs) in graphene can migrate when irradiated by electron beams from a transmission electron microscope (TEM). Here, we present an ab initio study on the atomic scale mechanism for the GB motion with misorientation angle of 30 in graphene. From total energy calculations and energy barrier calculations, we find that a Stone–Wales(SW)-type transformation can occur more easily near GBs than in pristine graphene due to a reduced energy barrier. There are other cases of migration which can be understood by other type of transformation, named evaporation of a carbon dimer. We also find that a mismatch in the crystalline orientation at GBs can drive the evaporation of a carbon dimer easily by greatly reducing the corresponding overall energy barrier. After evaporation of the carbon dimer, the GBs can be stabilized through a series of SW-type transformations that result in GB motion. The GB motion induced by evaporation of the dimer is in excellent agreement with recent TEM experiments.

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