## Mediator atoms drive structural evolution of defects in graphene

In a recent article in *Science Advances* (doi:10.1126/sciadv.aba4942), Gun-Do Lee of Seoul National University and co-workers reported the first direct observations of under-coordinated carbon atoms in mediating the structural evolution of defects in graphene. Their work provides valuable data for understanding defect transformation and growth in graphene and more broadly in two-dimensional nanomaterials.

Previously, it was revealed that under-coordinated atoms in graphene catalyze the breaking and formation of C–C bonds in graphene. The temporal and spatial resolution of conventional electron microscopy, however, has impeded elucidation of the precise role of these catalytic atoms during the structural change. Lee and co-workers tackled this challenge by using an advanced transmission electron microscope (TEM) equipped with an aberration corrector and a double Wien filter monochromator, achieving sub-angstrom resolution. With the aid of this state-of-the-art instrument, the researchers were able to observe how the under-coordinated atoms, coined "mediator atoms," regulated the structural evolution of defects in graphene.

The researchers explored the dynamics of the mediators by analyzing enormous numbers of TEM images for over a year. Generated at defective zones such as grain boundaries and dislocations, mediator atoms can hop into nearby point defects and embed themselves in the local $sp^2$-carbon network. The addition of these foreign atoms perturbs the local $sp^2$-network and induces the evolution of new, stable structures through breaking, formation, and switching of C–C bonds. These changes terminate after the mediator atoms are either stabilized in the graphene network, are kicked out of the graphene plane, or are quenched with other mediator atoms.

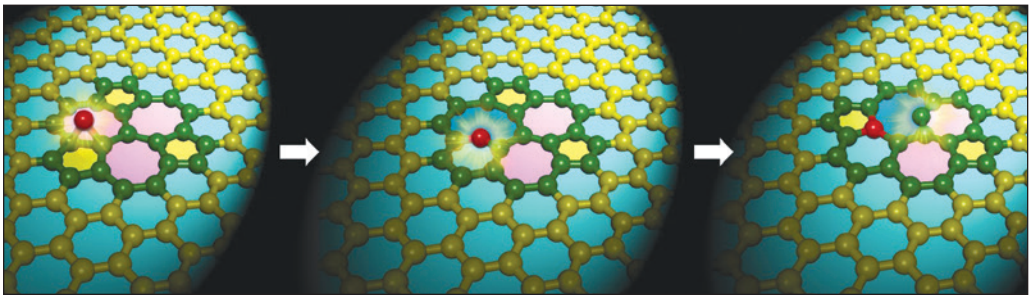
Additionally, the researchers studied the structural evolution by simulation techniques, including molecular dynamics simulations and density functional theory. The mediator-atom mechanism nicely reproduced the experimental microscope images and showed energy barriers lower than 2.0 eV (mostly below 1.0 eV). These energy barriers are much smaller than those predicted by the Stone–Thrower–Wales mechanism commonly accepted for explaining the evolution of graphene defects.

Boris I. Yakobson, a materials physicist at Rice University, says, "An impressive mix of state-of-the-art, high-resolution microscopy and atomistic simulations shows, in real-time, the transient morphology evolution of defects mediated by extra atoms. My group has theorized about such 'radical-dislocations' mobility in $MoS_2$, so I am particularly intrigued seeing it for the first time. I almost want to say '*in vivo*,' as if stiff graphene is alive at these conditions—warm and under the beam." Yakobson was not involved in this study.

Lee says that the concept of the mediator-induced structural evolution applies to other two-dimensional materials, for example, $MoS_2$ and $WS_2$, as well as three-dimensional (3D) materials. For 3D compounds, "it is difficult to observe the mediating phenomenon because point defects such as under-coordinated atoms can overlap with other atoms along the observation direction," Lee says.

Lee also envisions that "future studies of structural transformation by mediator atoms will become more vigorous both experimentally and theoretically."

**Tianyu Liu**



A mediator atom (red) alters five-membered (yellow) and seven-membered (pink) rings into six-membered (light blue) and eight-membered rings (dark blue) in a graphene network. Credit: Gun-Do Lee.





https://doi.org/10.1557/mrs.2020.217 Published online by Cambridge University Press