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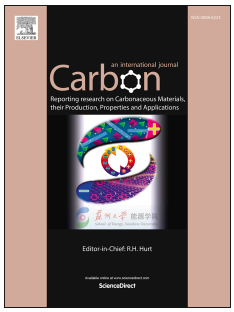

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Reaction Kinetics of Bond Rotations in Graphene

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Abstract

The formation and healing processes of the fundamental topological defect in graphitic materials, the Stone-Wales (SW) defect, are brought into a chemical context by considering the rotation of a carbon-carbon bond as chemical reaction. We investigate the rates and mechanisms of these SW transformations in graphene at the atomic scale using transmission electron microscopy. We develop a statistical atomic kinetics formalism, using direct observations obtained under different conditions to determine key kinetic parameters of the reactions. Based on the obtained statistics we quantify thermally and irradiation induced routes, identifying a thermal process of healing with an activation energy consistent with predicted adatom catalysed mechanisms. We discover exceptionally high rates for irradiation induced SW healing, incompatible with the previously assumed mechanism of direct knock-on damage and indicating the presence of an efficient nonadiabatic coupling healing mechanism involving beam induced electronic excitations of the SW defect.

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