Graphene oxide reduction under ultrafast laser irradiation: insights from reactive molecular dynamics

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At temperatures exceeding T=800–1000 K and in the presence of oxygen pure carbon undergoes rapid combustion. Nevertheless, recent experimental results on nanosecond laser irradiation of GO demonstrate that after heating up to 3000–3500 K this material transforms into graphene with high local order [1]. To shed light on the mechanisms behind this surprising effect we perform molecular dynamics modeling of GO reduction under high temperature conditions.

Our results [2] demonstrate that ultrafast heating produced by nanosecond laser combined with a fast cooling (the result of an extraordinary heat conductivity of graphene) leads to a fascinating regime of almost oxygen-free GO reduction in the air at T=2500–3500 K. While on the edges of GO at such temperatures we observe combustion process that captures atmospheric oxygen into CO and CO_2 molecules, central regions of GO undergoes rapid reduction and annealing with only little signs of oxidation. As a result, after a small loss of mass (primarily from its edges), GO transforms into graphene with a high local ordering.

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[2] Orekhov N D, Bondareva J, Potapov D O, Dyakonov P V, Dubinin O N, Diudbin G D, Maslakov K I, Logunov M A, Kvashnin D G and Evlashin S A *Carbon (in press)*