Atomic-scale description of electron beam damage in nitrogen-doped graphene and carbon nanotubes

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By combining state-of-the-art electron microscopy [1] with ab initio simulations [2], we study the mechanism of electron beam damage in nitrogen-doped graphene and carbon nanotubes. We show that the incorporation of nitrogen heteroatoms results in noticeable knock-on damage in these structures already at an acceleration voltage of 80 kV. Contrary to an earlier estimate predicting their rapid destruction via sputtering of the nitrogen atoms [3], our graphene results show that damage initiates by first displacing carbon atoms neighboring the nitrogen dopant, leading to the conversion of substitutional dopant sites into pyridinic ones. We estimate that acceleration voltages lower than 70 kV are required to avoid such damage. Besides providing an improved understanding of the irradiation stability of these structures, our results show that the possibility of structural changes cannot be neglected in characterization experiments employing high-energy electrons.

[1] J.C. Meyer et al., *Nature Materials* **10**, 209 (2011).
[2] J. Kotakoski et al., *ACS Nano* **6**, 671 (2012).
[3] T. Loponen et al., *Physical Review B* **74**, 073409 (2006).