Correction to Atomistic Description of Electron Beam Damage in Nitrogen-Doped Graphene and Single-Walled Carbon Nanotubes

[*ACS Nano* **2012,** *6*, 8837–8846. DOI: 10.1021/nn303944f]. Toma Susi,* Jani Kotakoski,* Raul Arenal, Simon Kurasch, Hua Jiang, Viera Skakalova, Odile Stephan, Arkady V. Krasheninnikov, Esko I. Kauppinen, Ute Kaiser,* and Jannik C. Meyer

An error was recently discovered in one of the references of our article.[1,2] This error affected the displacement cross sections calculated from displacement threshold energies, which were shown in the original Table 1 and Figure 1. In this erratum, we present the corrected values. The changes do not affect any of the conclusions of our article. Within the text, the only affected sentence is on page 8840, where a calculated cross section was said to be 0.03 barn. The corrected value is 0.21 barn, which is much closer to the experimental estimate of 0.16 barn.

TABLE 1. Influence of SWCNT Diameter (Fitted According to Figure 4 of the Original Article) on the Displacement Thresholds of Carbon or Nitrogen Atoms for Different Atomic Configurations (Figure 1)

target[a]	*d* (nm)	T_D (eV)	$\sigma_{80kV}^{-100\ °C}$ (barn)	σ_{100kV}^{RT} (barn)
C@N	1	18.5	0.42	5.36
	2	19.1	0.22	4.05
N@N	1	18.4	0.03	1.59
	2	19.0	0.01	1.00
C@1NV	1	18.3	0.52	5.85
	2	18.9	0.28	4.46
N@1NV	1	15.5	1.12	9.02
	2	16.0	0.66	7.07
N@2NV	1	16.0	0.66	7.07
	2	16.5	0.38	5.42
N@3NV	1	16.5	0.38	5.42
	2	17.1	0.18	3.83
N@4ND	1	16.0	0.66	7.07
	2	16.5	0.38	5.42
C[b]	1	21.5	0.01	0.97
	2	22.2	4.0×10^{-3}	0.58
C@SV[b]	1	14.2	10.7	22.1
	2	14.6	8.63	20.0
C@DV[b]	1	15.6	4.75	15.2
	2	16.1	3.38	13.1

[a] Target atom @ dopant configuration; SWCNT diameter for threshold fitting *d*; calculated displacement threshold T_D; cross sections (σ) at 80 kV (calculated at −100 °C) and 100 kV (at RT). [b] C, C@SV, and C@DV correspond to C atoms in ideal sp^2-bonded carbon and single and double vacancy configurations, respectively. The T_D values for C@SV and C@DV in graphene are from ref 3.

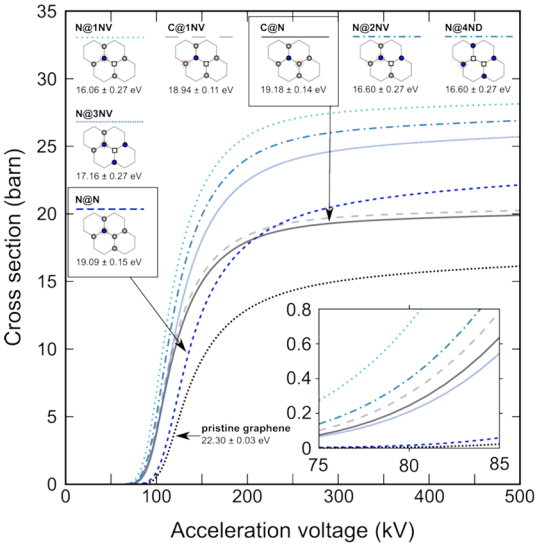

Figure 1. Calculated displacement thresholds and cross sections for different dopant configurations in graphene: substitution (labeled "N"), single pyridinic vacancy (1NV), double pyridinic vacancy (2NV), triple pyridinic vacancy (3NV), and quadruple pyridinic divacancy (4ND). In the schematic presentations, a dashed red circle marks the atom for which the threshold is calculated. Blue atoms denote nitrogen, gray ones carbon, and vacancies are marked by open squares. The cross sections calculated at RT are shown as a function of the acceleration voltage of the electrons, with the inset showing a higher magnification around 80 kV.

REFERENCES AND NOTES

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Published online July 15, 2013
10.1021/nn4034629