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Electronic Supplementary Information for "Structural Transformations of Carbon and Boron Nitride Nanoscrolls at High Impact Collisions"

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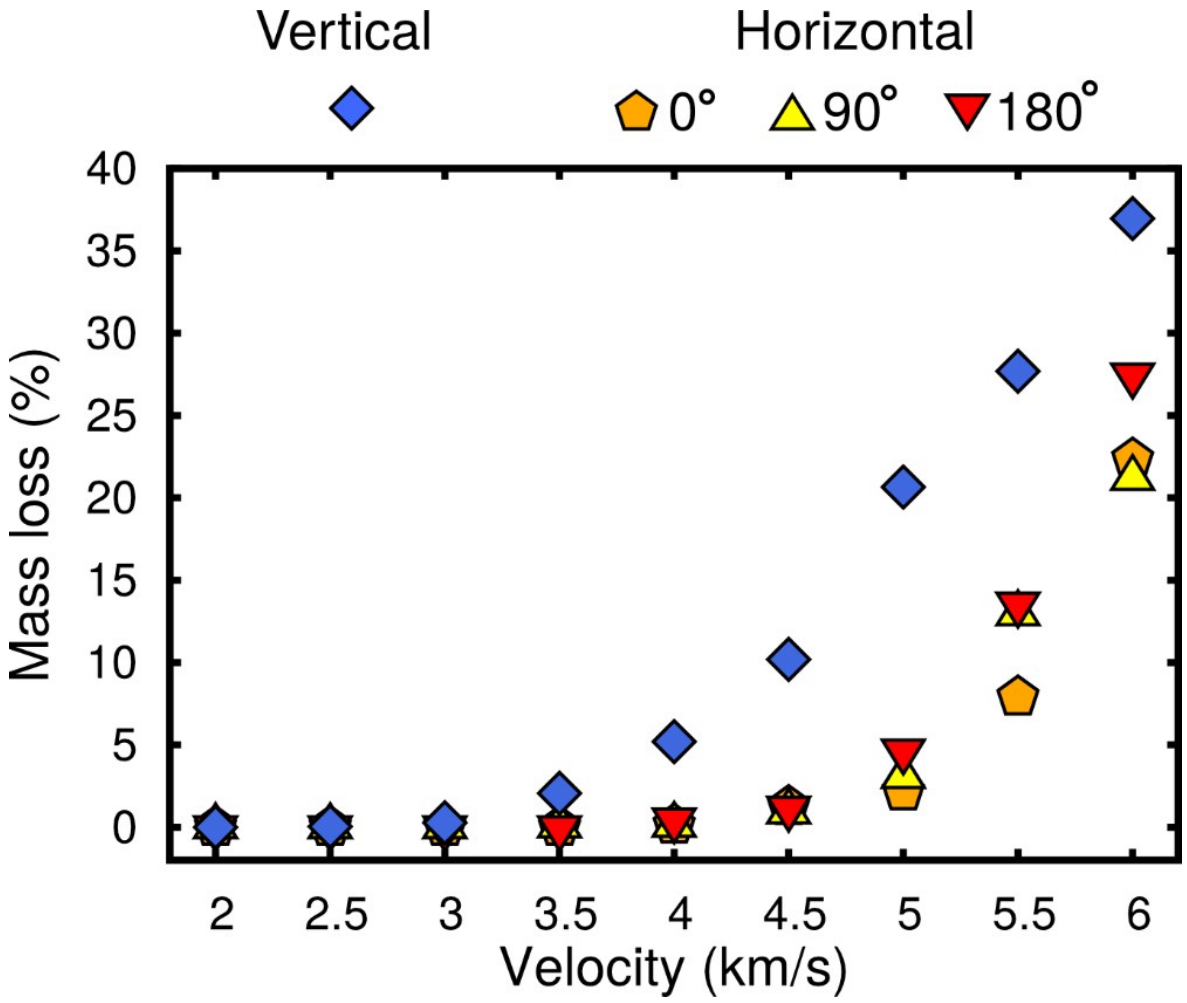

Figure S1: Mass loss percentage for carbon nanoscrolls colliding with a target at different velocities and impact orientations. For all tested velocities, more atoms are ejected at vertical impacts cases.

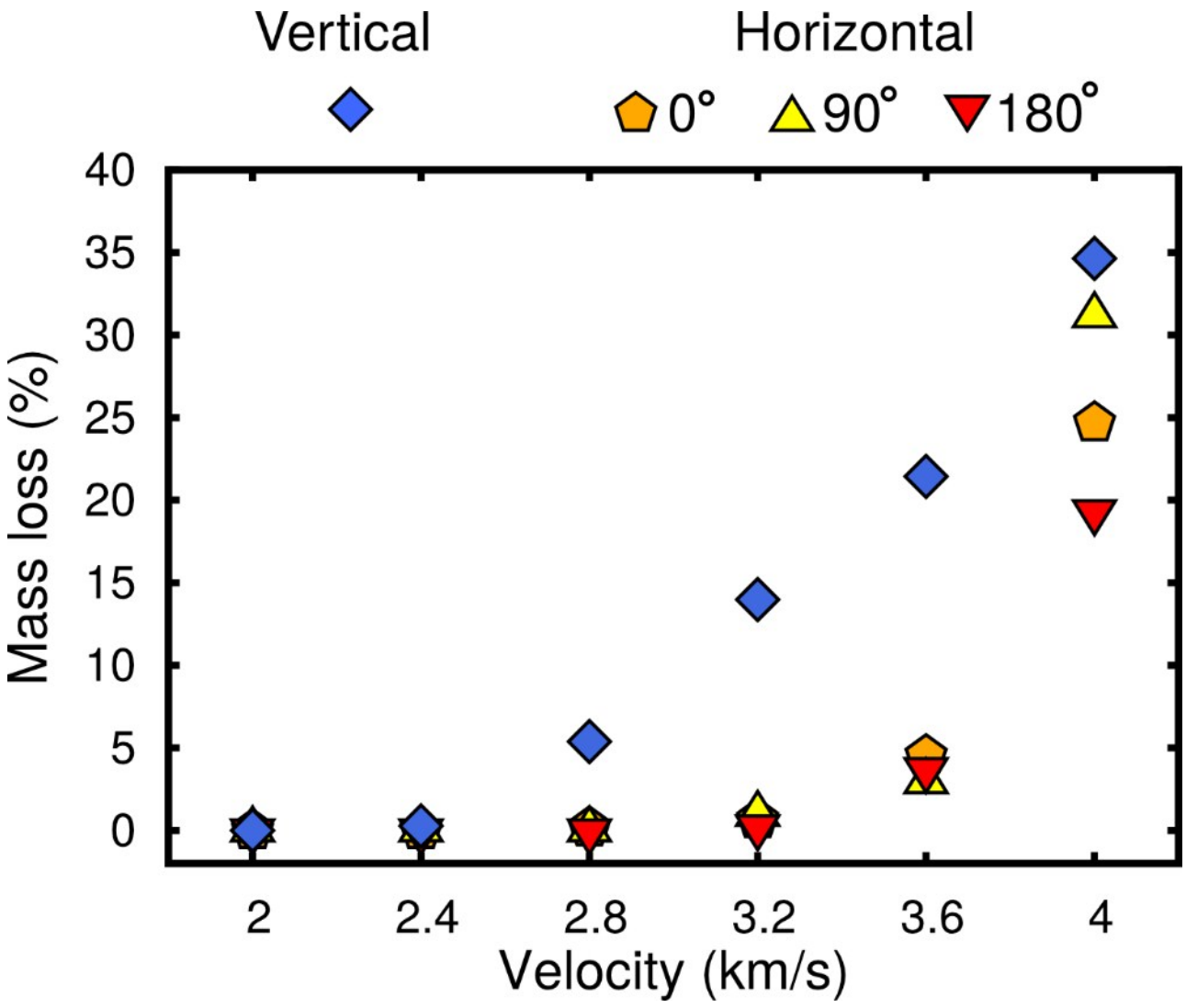

Figure S2: Mass loss percentage for h-BN nanoscrolls colliding with a target at different velocities and impact orientations. For a given impact velocity, BN scrolls eject more atoms than carbon ones.

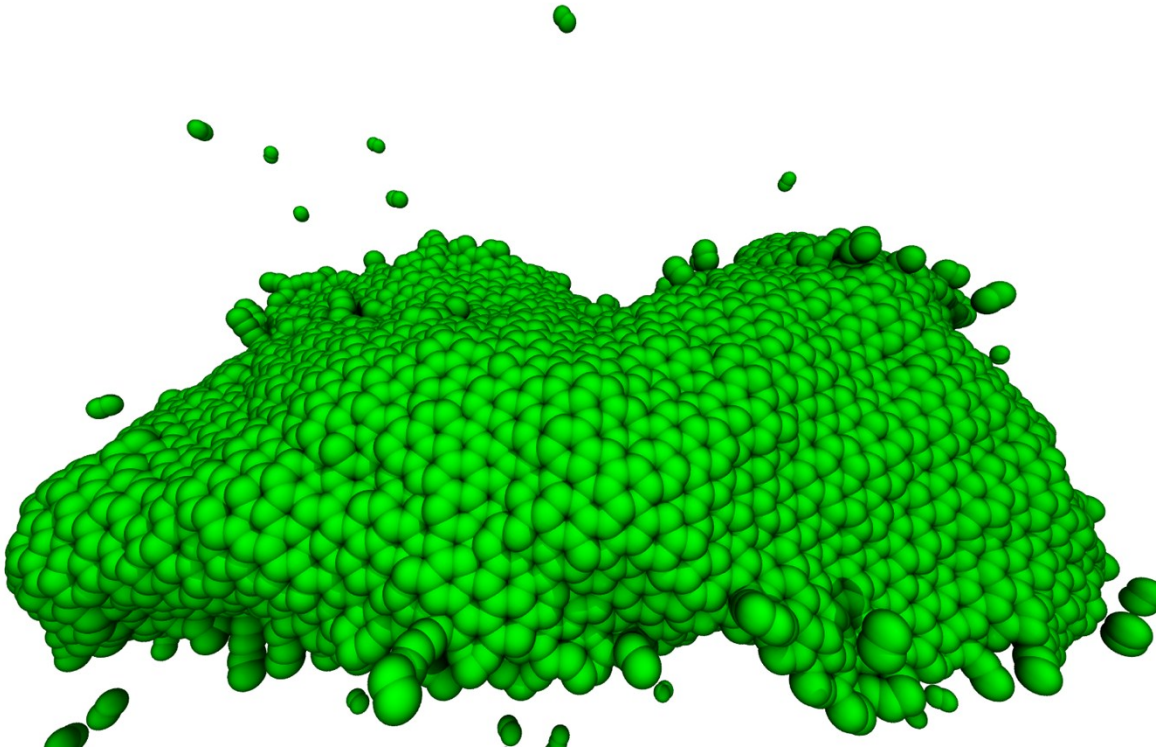

Figure S3: Representative molecular dynamics snapshot of a resulting amorphous structure after a lateral velocity impact of 5.5 km/s. In this case upper of this carbon nanoscroll side experiences little damage, while its lower side exhibits extensive damage – see the relevant frame of figure 3.

Relatives energies for all considered cases

TABLE S1: Potential energies for different carbon nanoscrolls collision orientations

Velocity (km/s)	Vertical Potential Energy Variation (10^4 kcal/mol)	Lateral 0° Potential Energy Variation (10^4 kcal/mol)	Lateral 90° Potential Energy Variation (10^4 kcal/mol)	Lateral 180° Potential Energy Variation (10^4 kcal/mol)
2.0	1.53	1.21	0.70	1.23
2.5	2.47	1.95	1.64	2.02
3.0	3.53	2.40	2.41	2.96
3.5	5.04	3.39	3.55	4.05
4.0	6.88	4.69	4.98	5.42
4.5	8.98	6.54	6.77	7.30
5.0	11.28	8.83	9.25	10.12
6.0	16.65	15.78	16.25	16.96

TABLE S2: Potential energies for different BN nanoscrolls collision orientation

Velocity (km/s)	Vertical Potential Energy Variation (10^4 kcal/mol)	Lateral 0° Potential Energy Variation (10^4 kcal/mol)	Lateral 90° Potential Energy Variation (10^4 kcal/mol)	Lateral 180° Potential Energy Variation (10^4 kcal/mol)
2.0	1.41	1.22	1.28	1.28
2.4	2.17	1.71	1.83	1.81
2.8	3.07	2.46	2.75	2.73
3.2	4.08	3.82	4.17	4.02
3.6	5.25	5.08	5.36	5.42
4.0	6.44	6.34	6.57	6.63

Chiralities dependence: Broken bonds and mass loss

TABLE S3: Broken bonds and mass loss for impact at 3km/s of zigzag and armchair carbon nanoscrolls

Carbon – 3.0 km/s	*Zigzag – Broken bonds (%)*	*Armchair – Broken bonds (%)*	*Zigzag – Mass loss (%)*	*Armchair – Mass loss(%)*
0°	-0.20	-0.79	0	0
90°	-0.21	-0.79	0	0
180°	-0.12	-0.37	0	0

TABLE S4: Broken bonds and mass loss for impact at 5km/s of zigzag and armchair carbon nanoscrolls

Carbon – 5.0 km/s	*Zigzag – Broken bonds (%)*	*Armchair – Broken bonds (%)*	*Zigzag – Mass loss (%)*	*Armchair – Mass loss(%)*
0°	3.1	5.8	5.2	2.2
90°	3.9	5.3	4.8	3.0
180°	6.2	5.8	4.6	4.7

TABLE S5: Broken bonds and mass loss for impact at 2km/s of zigzag and armchair bn nanoscrolls

BN – 2.0 km/s	*Zigzag – Broken bonds (%)*	*Armchair – Broken bonds (%)*	*Zigzag – Mass loss (%)*	*Armchair – Mass loss(%)*
0°	0.20	0.42	0	0.04
90°	0.11	0.34	0	0.24
180°	0.11	0.31	0	0.04

TABLE S6: Broken bonds and mass loss for impact at 3.2 km/s of zigzag and armchair bn nanoscrolls

BN– 3.2 km/s	*Zigzag – Broken bonds (%)*	*Armchair – Broken bonds (%)*	*Zigzag – Mass loss (%)*	*Armchair – Mass loss(%)*
0°	15.6	15.5	0.65	0.63
90°	20.5	17.2	0.94	0.74
180°	17.5	17.7	0.25	1.3

Chiralities dependence: Structural Transformations

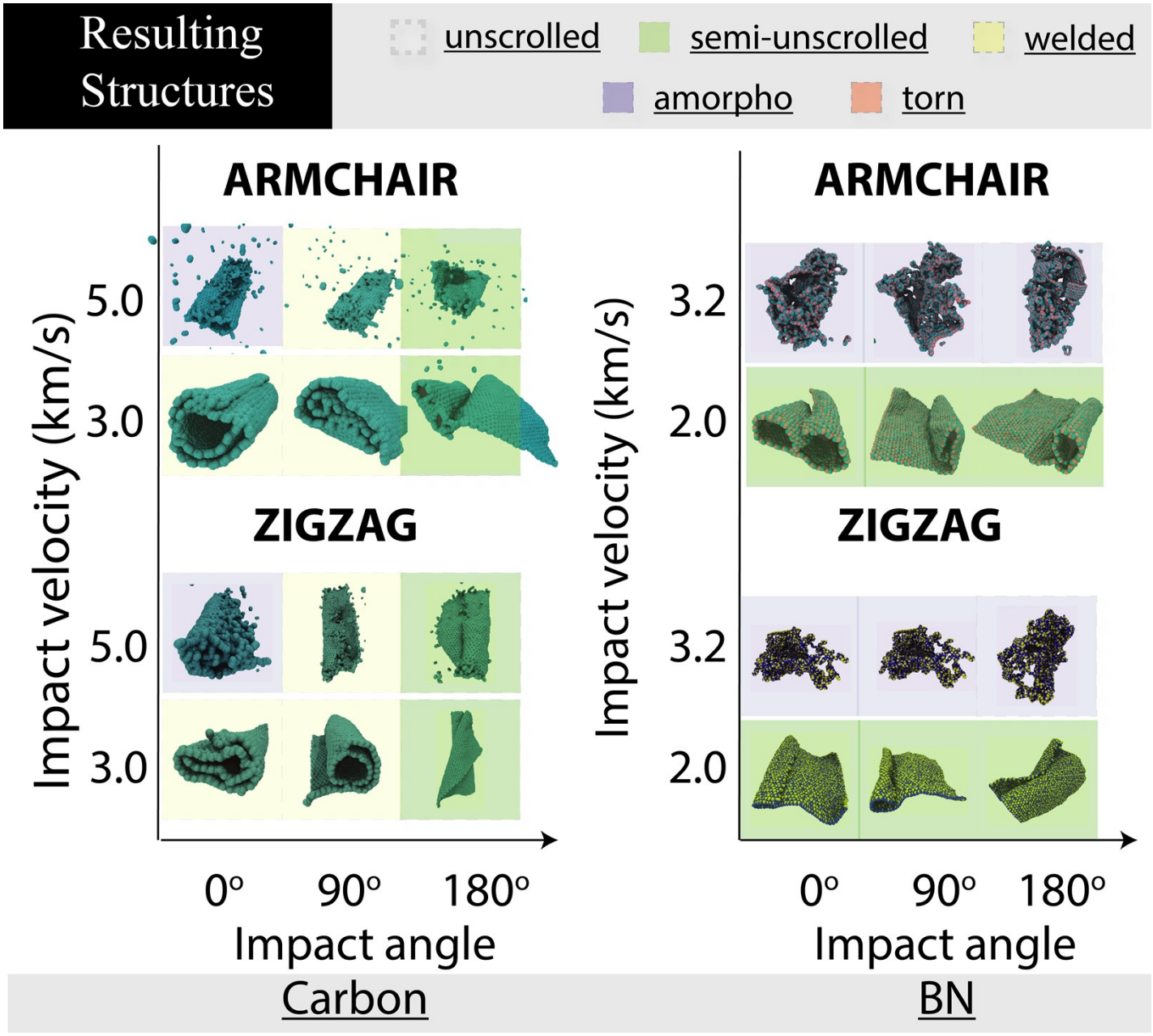

Figure S4: MD snapshots comparison between Armchair and Zigzag resulting structures after lateral scroll impacts, as a function of impact angle and velocity. Notice that snapshot orientation is unrelated to impact angle. For instance, many structures for α = 0o are depicted with their open edge upwards, but in the simulations, they were facing the target (downwards). We observed less bond reconstruction at impact when BN based nanoscrolls were employed, due to their brittle nature. Note that 1 km/s is equal to 10 Å/ps.