Experimental Observation of Boron Nitride Chains

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Supplementary information

- Formation of dual monoatomic chains

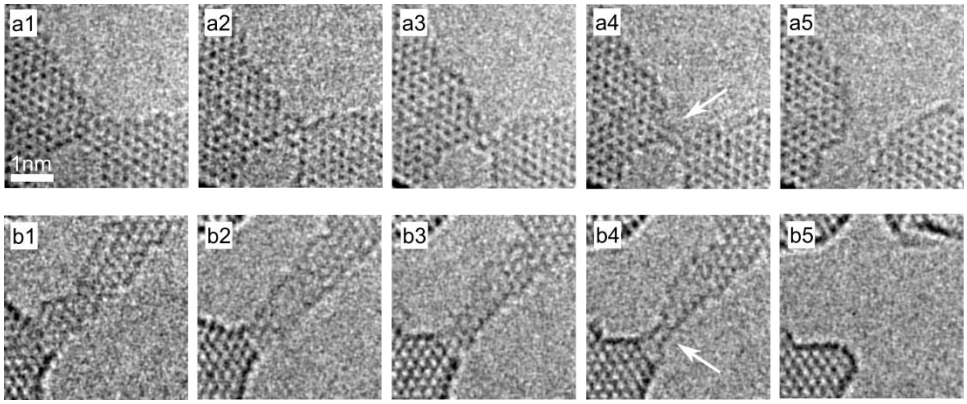

Figure S1 – Image sequences illustrating the formation of suspended dual monoatomic chains. The data was acquired using 60kV electrons, with the sample at 650°C. The images were processed with a median filter and contrast-enhanced for clarity.

- The interaction between supported BN chains and the supporting layer

The interaction of a BN chain with the pristine BN substrate or with a B/N vacancy were studied using a 5x5 supercell and 5 units of BN chain. Due to the small mismatch in periodicity, the BN chain is slightly bent. The binding energies were evaluated using the following formula: $E_{bind} = E_{total} - E_{substrate} - E_{pristinechain}$,yielding -0.58 eV or -0.12 eV/BN unit. In the case of chain interacting with B or N vacancy, there are a large number of possible configurations. In order to quickly sample the configuration space, we first ran MD at 300K for 1 ps and then relaxed the obtained structure. These are shown in Fig. S2. The binding energies are -3.50 eV and -0.85 eV for B and N vacancy, respectively. Subtracting the interaction with the pristine lattice, we obtain “additional” binding energies of -2.92 eV and -0.27 eV, per B and N vacancy, respectively.

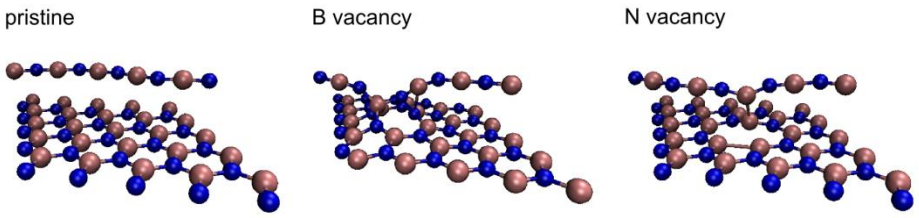

Figure S2 – Images of a supported BN chain after geometrical optimization with no defects (left), a B vacancy (middle) and a N vacancy (right) present on the supporting layer.

- The interaction between supported BN ribbons and the supporting layer

The interaction energies for ribbons oriented in different ways with respect to a substrate layer were calculated using the following formulas: $E_{flat}(n) = \gamma_{ZZB} + \gamma_{ZZN} - nE_{vdW}$ and $E_{stand}(n) = \gamma'_{ZZN(B)} + \gamma_{ZZB(N)}$, where γ and γ' are the edge energies for the flat and perpendicular case, respectively. The energies are plotted in Fig. S3. For ribbons consisting of 1-3 hexagons, standing vertically is energetically favored. This is due to the fact that the edges can interact strongly with the substrate in this orientation, while the van der Waals energy (E_{vdW}) vanishes. The case where the B-terminated zig-zag edge is attached to the substrate is the lowest in energy. For 1-hexagon wide ribbons, some configurations are stable, whereas some relax to BN chains. From the energy difference between the flat and standing configurations we obtain the interaction strength of the edge with the substrate, which reaches 0.84 eV for ZZN2 and 0.3-0.4 eV for ZZN3/ZZB3.

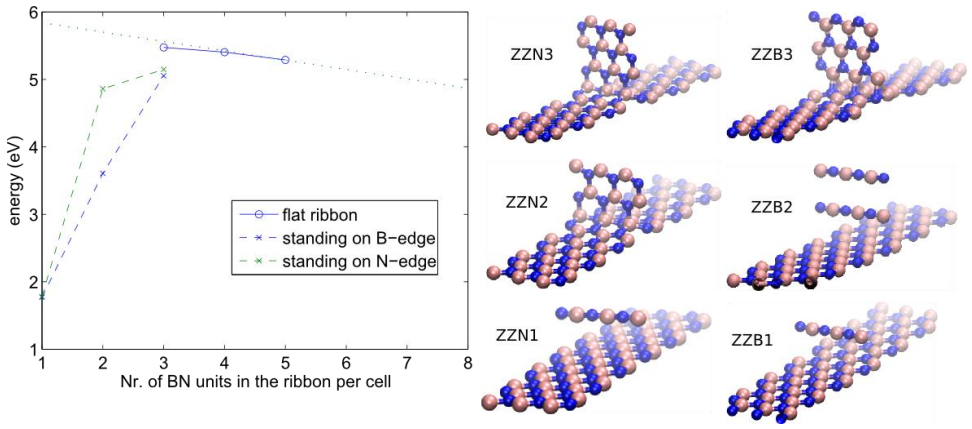

Figure S3 – Calculated interaction energy between BN nanoribbons of different sizes and the BN substrate that supports them (left) and models for the first few ribbons considered (right).

- The evolution of open-ended supported monoatomic chains

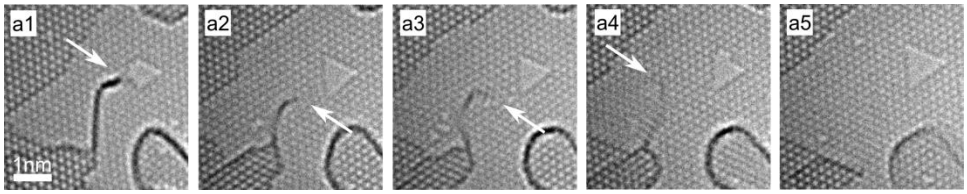

Figure S4 – Image sequence showing the evolution of an open-ended supported monoatomic chain. The data was acquired using 80kV electrons, with the sample at 20°C. The images were contrast-enhanced for clarity.

- Damage creation in BN by sub-threshold irradiation

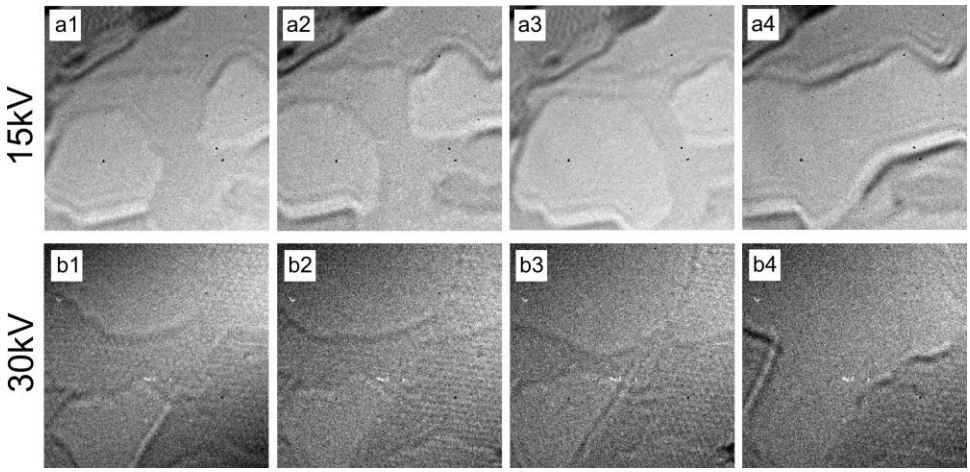

Figure S5 – Image sequences illustrating the progressive damaging of h-BN due to 15kV and 30kV electron irradiation at 650°C.