

Supplementary Information

Seeking borophene on Ni₃Al(111): boron segregation and oxidation.

Y.Y. Grisan Qiu¹, P. Biasin¹, P. Mantegazza¹, S. Baronio¹, M. Heinrich^{2,3}, M.K. Muntwiler²,
and E. Vesselli^{1,4,5,*}

¹Department of Physics, University of Trieste, 34127 Trieste, Italy.

²Paul Scherrer Institut, Villigen, 5232, Switzerland.

³Swiss Nanoscience Institute, University of Basel, 4056 Basel, Switzerland.

⁴CNR-IOM, Istituto Officina dei Materiali, 34149 Trieste, Italy.

⁵Center for Energy, Environment and Transport Giacomo Ciamician, University of Trieste, 34127 Trieste, Italy.

*E-mail: vesselli@iom.cnr.it – evesselli@units.it

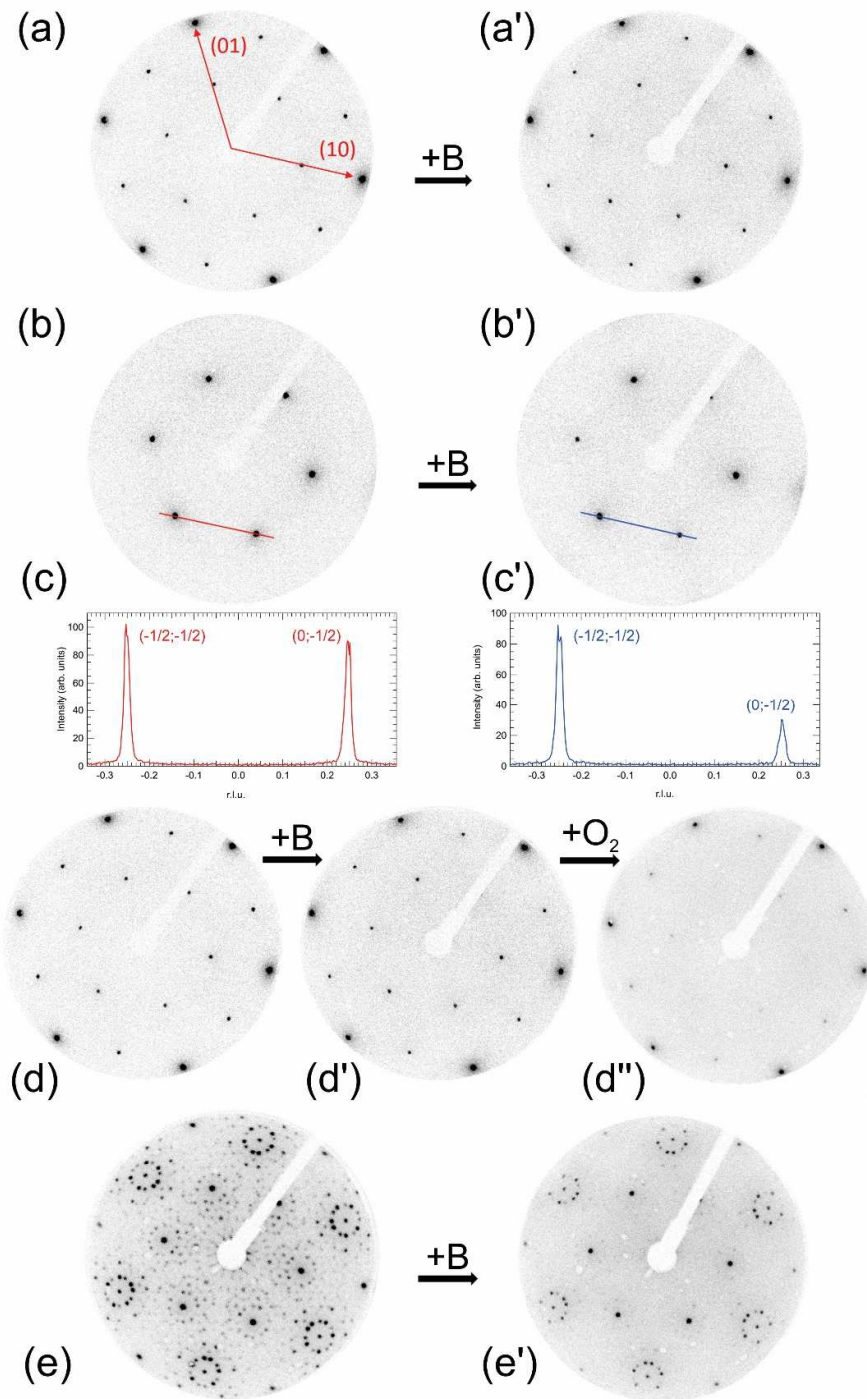


Figure S1. LEED characterization of the B/Ni₃Al(111) layers: (a,b) diffraction images collected at room temperature from the clean Ni₃Al(111) termination at 60 and 47 eV, respectively, compared to the corresponding patterns (a',b') after deposition of 2 ML of B at 500 K with a rate of 0.05 ML/min; (c,c') diffraction spot profiles along the lines depicted in (c,c'), respectively; (d,d',d'') from left to right, clean Ni₃Al(111), pristine 2 ML B/Ni₃Al(111) and after oxidation with 12 L O₂ at room temperature (E = 60 eV); (e) pristine ultrathin Al₂O₃/Ni₃Al(111) oxide film (E = 60 eV); (e') 2 ML B/Al₂O₃/Ni₃Al(111) (E = 60 eV).

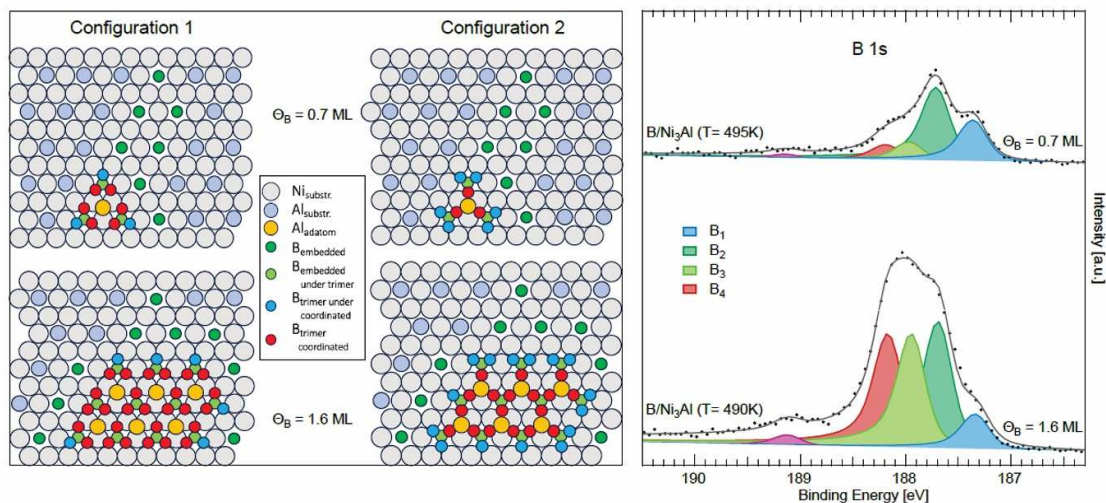


Figure S2. Left: Interpretative model of Configurations 1 and 2, both at low coverage ($\Theta_B = 0.7$ ML, top) and high coverage ($\Theta_B = 1.6$ ML, bottom). The substrate is composed by Ni and Al atoms (grey and light blue, respectively). B atoms replace Al atoms to form the B-embedded substrate (dark green). The triangular protrusions are characterized by three trimers of boron atoms (cyan and red) arranged above a substitutional B atom (light green) and connected by an Al adatom (yellow). Right: XPS measurements of B 1s core-level spectra at low coverage ($\Theta_B = 0.7$ ML, top) and high coverage ($\Theta_B = 1.6$ ML, bottom).

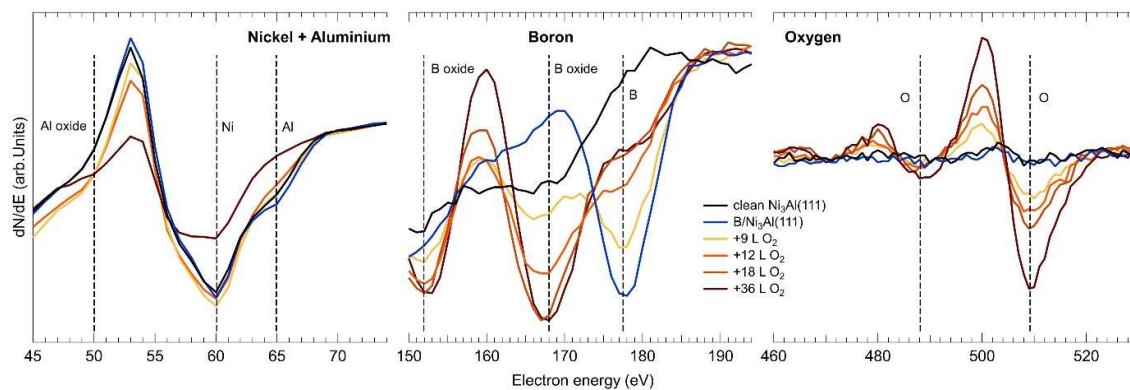


Figure S3. Auger spectra (primary electrons energy 3 keV) of the clean $\text{Ni}_3\text{Al}(111)$ surface (black lines) after deposition of 2 ML B at 500 K (blue) and for increasing oxidation exposures at room temperature (see color legend) collected in the Ni and Al (left), B (center) and O (right) transitions regions.