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Citation for the original published paper (version of record):
Mohammed Idris Bakhit, A., Ali, K., Makarova, A. et al (2022). Structure and electronic properties of stable facets in the 2D material hexagonal boron nitride
(hBN) on curved platinum. Science Talks, 4. http://dx.doi.org/10.1016/j.sctalk.2022.100071

Science Talks 4 (2022) 100071

Contents lists available at ScienceDirect

Science Talks

journal homepage: www.elsevier.es/sctalk

Structure and electronic properties of stable facets in the 2D material hexagonal boron nitride (hBN) on curved platinum

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ARTICLE INFO

Keywords:
Hexagonal boron nitride (h-BN) monolayer
2D materials
Epitaxy
Curved crystal
Stable facets

ABSTRACT

A hexagonal boron nitride (hBN) monolayer was grown on a curved crystal c-Pt(331) substrate including all vicinal surfaces between Pt(111) and Pt(110) faces. The surface structure has been studied by a combination of low-energy electron diffraction (LEED) and scanning tunnelling microscopy (STM). We observed that the hBN monolayer covers the entire curved crystal, but induces a faceting subsequent to the growth. We encountered (111), (221), (441), (991), and (110) as stable facets. We assign this faceting to two factors i) a better lattice coincidence and ii) the existence of local covalent bonds and non-local Van der Waals interactions.
The electronic structure was characterized by near-edge x-ray absorption fine structure (NEXAFS), X-ray photoemission spectroscopy and angle-resolved photoemission spectroscopy (ARPES). The hBN/Pt(111) has the weakest interacting overlayer system, while the hBN on vicinal surfaces is more strongly bound to the Pt substrate.
Additionally, we determined using angle-resolved photoemission measurements (ARPES) that the π band shifts downward when going away from the hBN/Pt(111) surface towards hBN/Pt(110). In the latter case, the π band shift is the largest.

Video to this article can be found online at https://doi.org/10.1016/j.sctalk.2022.100071.

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http://dx.doi.org/10.1016/j.sctalk.2022.100071
Received 10 August 2022Accepted 15 August 2022

Figures and tables

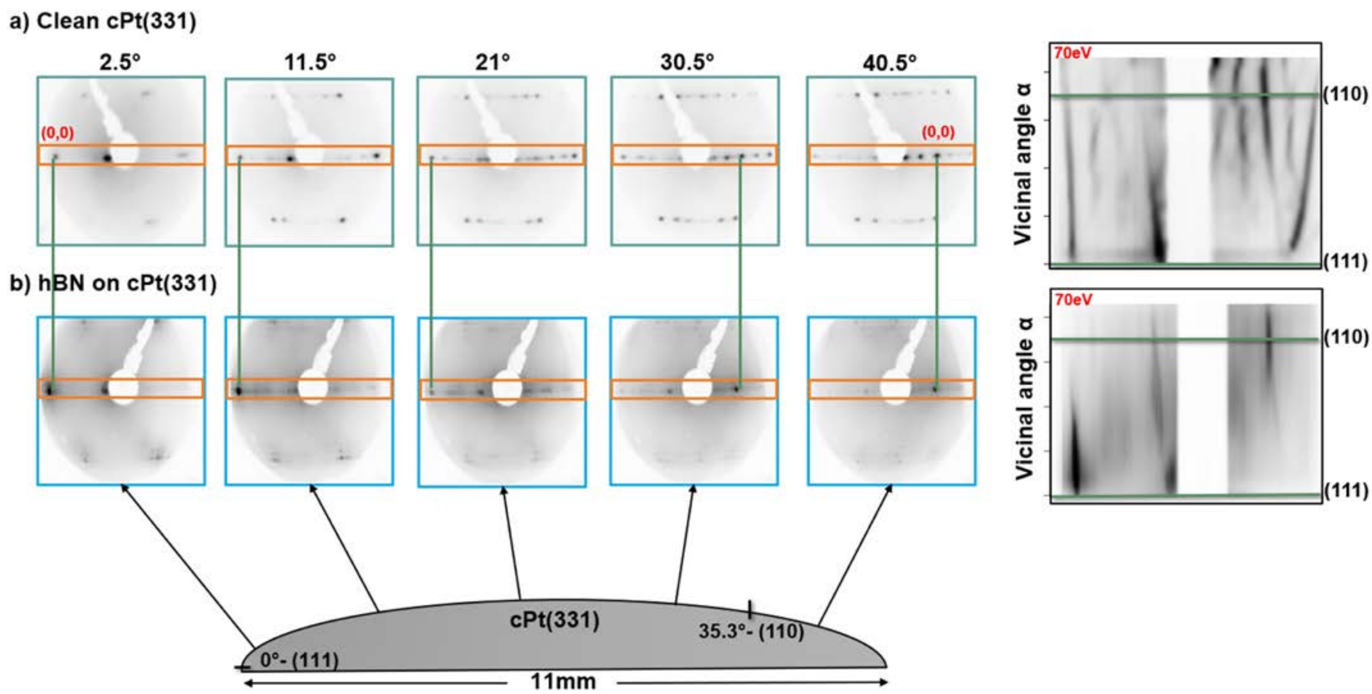

Fig. 1. Evolution of the Low Energy Electron Diffraction (LEED) patterns of platinum (a) and hBN covered platinum (b) along the curved Pt(331) surface as a function of the vicinal angle. The right-hand images display the intensity variations of the central horizontal rectangle. One observes crossing features in (a) due to the continuous increase of the terrace width in pure Pt and parallel features in (b) due to the facet formation. The kinetic energy of the electrons was set to 70 eV.

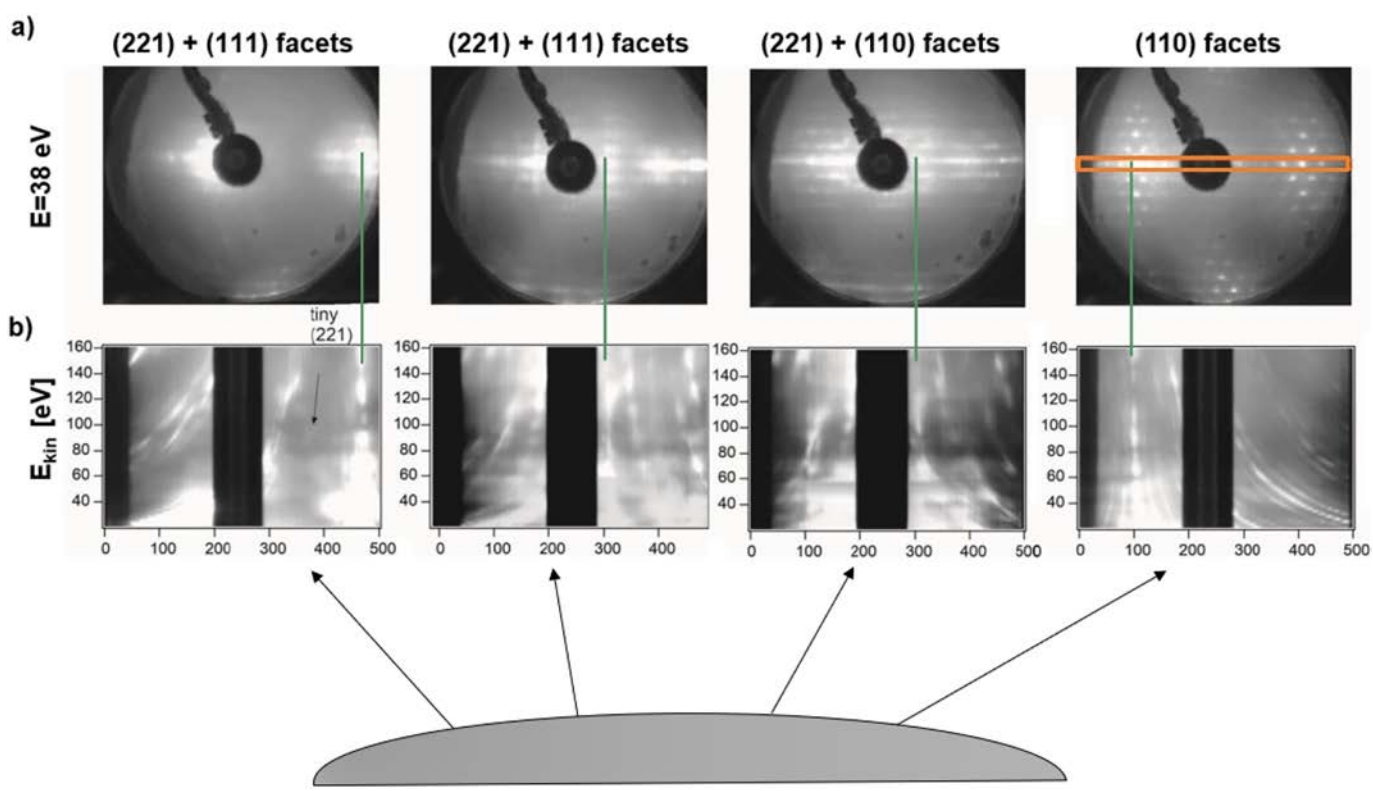

Fig. 2. LEED IV Analysis of hBN grown on curved Pt(331): (a) LEED pattern at the indicated positions taken at E_{kin} = 38 eV. (b) LEED IV image profile was taken at the central line indicated by the orange rectangle. The green lines denote the (0,0) spots of the stable facets that are indicated at the top.

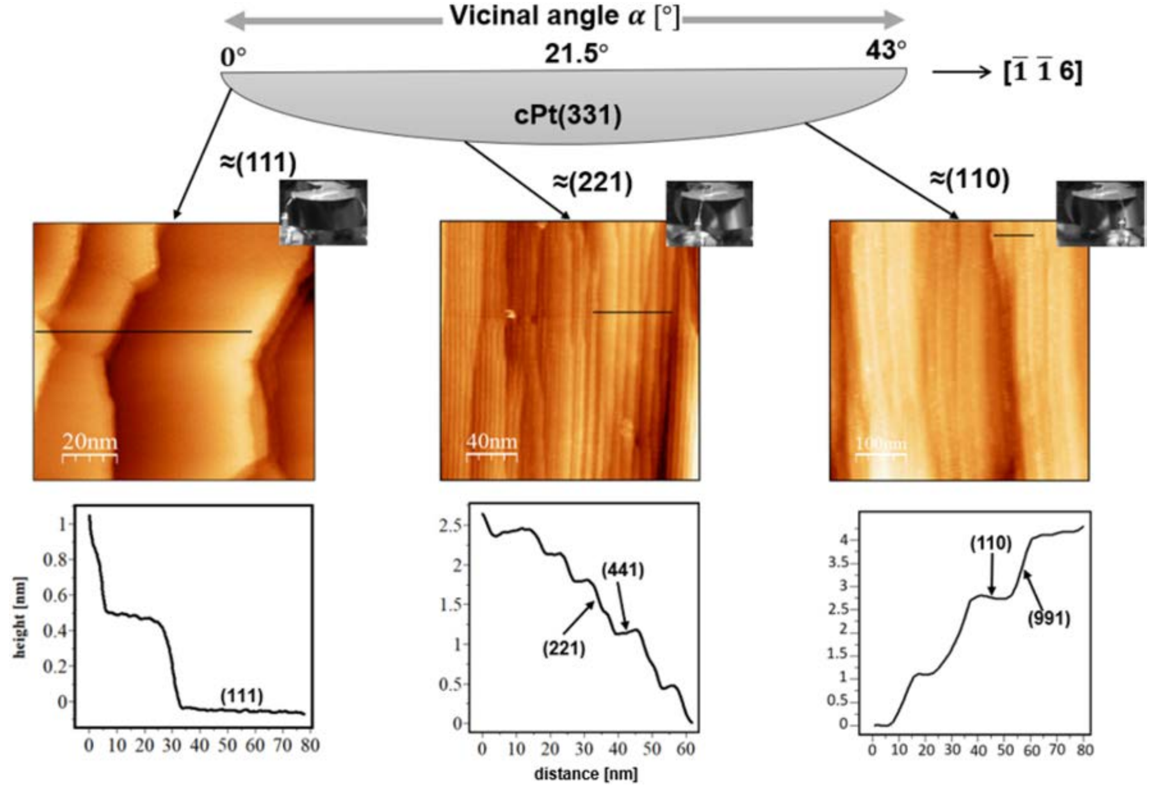

Fig. 3. Scanning Tunnelling Microscopy (STM) images of hBN-covered c-Pt(331) at different positions of the curved substrate (U_{bias} = 1 V, I = 2 nA). The bottom panels indicate the height profiles for the indicated black lines in the STM images.

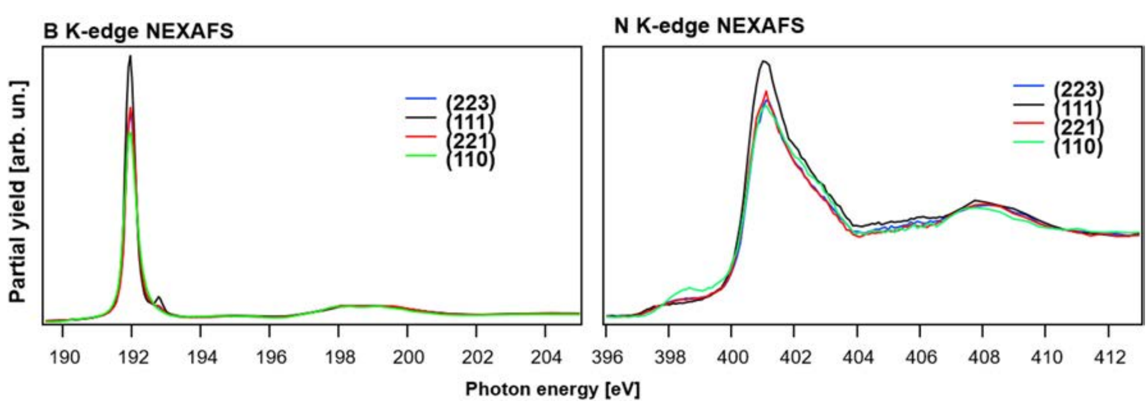

Fig. 4. X-ray absorption (XAS) of the K-edges of B and N at different positions of the curved c-Pt(331) crystal after hBN growth.

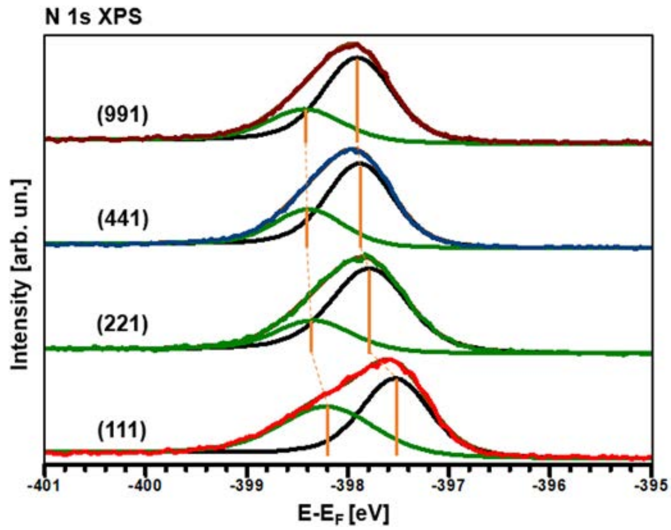

Fig. 5. X-ray photoemission spectroscopy (XPS) of the N 1 s core level of hBN/c-Pt(331) at different positions of the curved substrate. The photon energy was 480 eV, and the measurements were taken at 300 K.

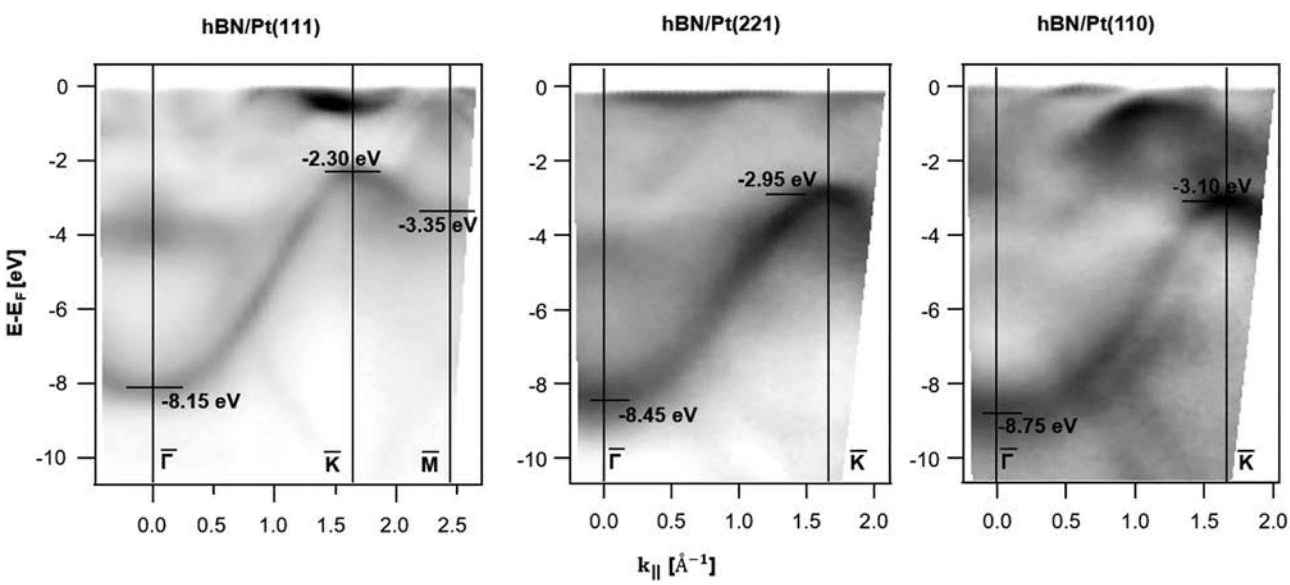

Fig. 6. Angle-resolved photoemission spectroscopy (ARPES) intensity mappings along the $\overline{\Gamma}$ - $\overline{K}$- $\overline{M}$ direction of the surface Brillouin zone of the hBN-covered surfaces at the stable facet positions (111), (221) and (110).

CRediT authorship contribution statement

Alaa Mohammed Idris Bakhit: Data analysis**,** Writing- Original draft preparation, Visualization, Software, Experimental work. **Khadiza Ali:** Data collection, Methodology, Investigation, Experimental work. **Anna A. Makarova:** Experimental work. **Igor Piš:** Experimental work. **Federica Bondino:** Experimental work. **Frederik Schiller:** Supervision, Validation, Investigation, Conceptualization, Writing- Reviewing and Editing.

Acknowledgements

We acknowledge financial support from grant PID2020-116093RB-C44 funded by the Spanish MCIN/AEI/10.13039/501100011033, as well as the Basque Government Grant IT-1591-22. The research leading to this result has been further supported by the project CALIPSOplus under Grant Agreement 730872 from the EU Framework Programme for Research Innovation HORIZON 2020. A.A.M. acknowledge BMBF (grant no. 05K19KER).

Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Further reading

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She graduated from the Sudan University of Science and Technology, Sudan. She acquired a master's in mathematical sciences from AIMS-Cameroon, Cameroon. Additionally, she earned a master's degree in condensed matter physics from the East African Institute for Fundamental Research (ICTP-EAIFR), Rwanda. Currently, her PhD project is focused on the growth of 2D materials hexagonal boron nitride (hBN) on different curve crystal substrates, studying the structure and electronic properties using experimental techniques and theoretical methods.

Khadiza Ali received her PhD from TIFR (Mumbai, India) in 2018 and spent the next 3 years in CFM-MPC (San Sebastian, Spain) exploring the growth and electronic structure of hBN and graphene on curved crystals. Currently, Khadiza is a postdoctoral researcher at Chalmers university of technology (Gothenburg, Sweden). Her main expertise is in investigating functional materials using angle-resolved photoelectron spectroscopy and X-ray photoelectron spectroscopy.

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