Understanding the nucleation and growth of borophene on substrate using Machine Learning Tools

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Single layer materials have drawn a lot of attention due to their peculiar physical properties (opto-electronic properties, high conductivity, flexibility…). In particular, it has been predicted that boron could exist as a single atomic layer in distinctive crystallographic configurations (allotropes), called *borophene* – in reference to the carbon equivalent, graphene. Borophene is one of the only 2D material with metallic behaviour, among other interesting properties [1]. Recent studies have focused on the synthesis of such material under various allotropic forms, the obtained allotrope depending on the substrate used and experimental parameters such as synthesis temperature [2–5]. However, the link between the various synthesis parameters and the obtained allotrope is still unclear. To be able to control the synthesis of allotropes selected for their wanted properties, one needs a good understanding of the growth mechanisms and phase transitions at stake in this system. Therefore, a strong theoretical support is needed, with accurate reactive simulations of large systems. However, while ab initio simulations are accurate, they are slow and do not allow studying large systems – and classical Molecular Dynamics require a force field that is not available for this system.

In recent works [6,7], we have developed a new reactive Machine Learned Interaction potential (MLIP) [8–10], which allows us to explore multiple structural arrangements of borophene allotropes on metal substrates. The developed MLIP presents the advantage of performing fast simulations with a level of accuracy comparable to ab initio calculations [11].

Using this new MLIP, we have studied the stability, nucleation and growth of borophene layers on top of a silver substrate using a blend of molecular dynamics and grand canonical Monte Carlo (GCMC) simulations – the latter is used to account for experimental parameters such as growth pressure and temperature while allowing growth of the system. Here again, we used machine learning tools to allow identifying the allotropic structures encountered during the simulations. A random forest classifier is trained on a collection of atomic environment descriptors, which allows attributing each atom and vacancies to their corresponding allotrope (Figure 1).

In the end, we are able to describe a relative stability scale for the various allotropes, as well as assessing the ones that favour growth. This leads us to identify stable and transitory states, as well as existence domains for several allotropes, in good agreement with experimental results.

References

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Figures

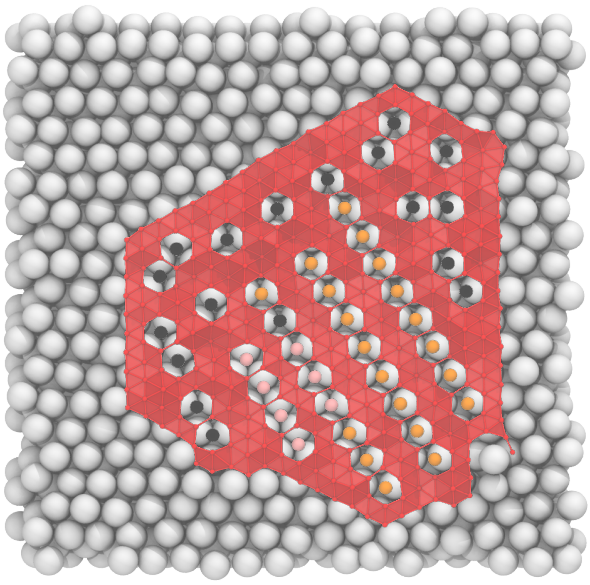

Figure 1. Snapshot of a borophene island (red) during growth on silver (grey spheres). The vacancies defining an allotrope are color attributed: pink for chi3, orange for beta12, black for un-attributed.