Adhesion model of graphene islands on metal substrates based on Moiré-patterns

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One problematic aspect of graphene (GR) CVD growth on metal substrates is that GR is capable to create rotational domains [1], separated by grain boundaries (GBs), sometimes even on a single crystal surface [2]. GBs worsen the electric properties of GR [3], therefore the nucleation of differently orientated islands is an undesirable phenomenon.

An interesting feature is, that the different existing orientations are very specific to the substrate (e.g: on Cu(111) the most commonly known orientations are: R0°, R7°, but for Ir(111) we have R0°, R14°, R19°, R23°, R26°, R30°)[4]. Even today there is no such a physical model that can somehow clarify the very basic nature of these orientations. Why only these orientations can appear, and what are the circumstances that influences the GR to realize one or another?

In order to understand these aspects we developed a continuum mathematical model that calculates the adhesion energy of a GR island with a given size and orientation only by knowing the underlying Moiré-pattern that is formed between the atomic lattices. This approach agrees surprisingly well with DFT and CMD results. This shows that we have captured some very basic physical insights of the adhesion.

Using our model, Monte-Carlo (MC) simulations can be carried out to perform GR growth simulations on several germs to analyze their distribution of orientation. These MC simulations are several orders of magnitude faster than Kinetic MC methods.

References

[1] M. Batzill, Surf. Sci. Rep. 67, (2012), 83.

[2] Li Gao et al., Nano Letters 10(9) (2010), 3512-3516.

[3] Vancsó, Péter, et al., Applied Surface Science 291,(2014), 58-63

[4] Tetlow, H., et al., Physics Reports 542.3 (2014), 195-295

Figures

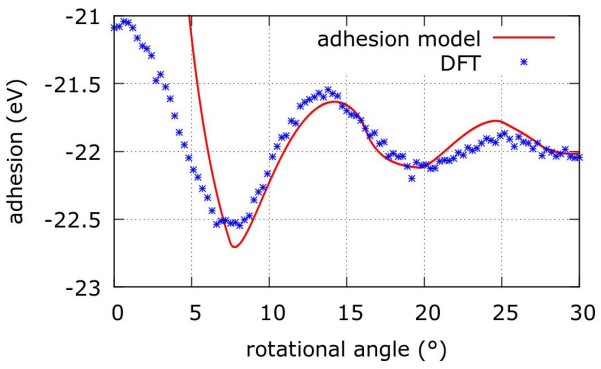

Figure 1: The dependence of the adhesion on the orientation of a GR nanoisland with a diameter of 2.2nm on Cu(111) surface. Our model (red line) is compared to DFT calculations (blue spots).