Moiré patterns formed by hexagonal coincidence lattices: applications for metal supported graphene and related materials

Sebastian Günther
Chemie Department, Technische Universität München, Lichtenbergstr. 4, D-85748 Garching

email: sebastian.guenther@tum.de

The current interest in graphene (g) and similar 2-dim materials supported on transition metal (TM) surfaces has raised again an old question: "Which moiré phases are observed when placing hexagonally arranged overlayers on hexagonally packed surfaces?" Especially the question occurs, whether or not moiré phases are commensurate and if so, what is the size and the correct indexing of their unit cell. Usually, trial and error methods are used to solve these questions. While for supported g an analytical description could be applied for a special case,[1-2] we derived a geometric construction in a more general way identifying spatial beating frequencies generated by two coinciding and arbitrarily oriented hexagonal lattices.[3] Our analysis delivers solvable analytic equations that predict whether or not first or higher order commensurability may occur which can be visualized as shown in Fig. 1. The displayed graphs indicate where commensurability of 1st and 2nd order spatial beating frequencies may occur within the parameter space of moirés that apply to g/Pt(111). The left axis represents the lattice constant ratio *x* and the horizontal axis the rotational angle φ of the two coinciding lattices. Yellow patches indicate, where true commensurability is reached. The unit cell can be indexed by a vector $(m,n)_{TM}$ relating to the TM- support lattice (TM=Pt(111)) and at the same time by a vector $(r,s)_g$ relating to the graphene lattice. The colored curves sketched in red/dark-blue ($(m,n)_{TM}$) and green/light-blue ($(r,s)_g$) represent the solutions of an analytical expression that leads to the correct indexing. Where such lines cross each other, commensurate cells can be observed as shown for the reported R19.2° and the R23.4° moirés of g/Pt(111). Our approach is universal and may be used for the description of moiré patterns formed on other hexagonally arranged thin layers on any hexagonally packed support surface.

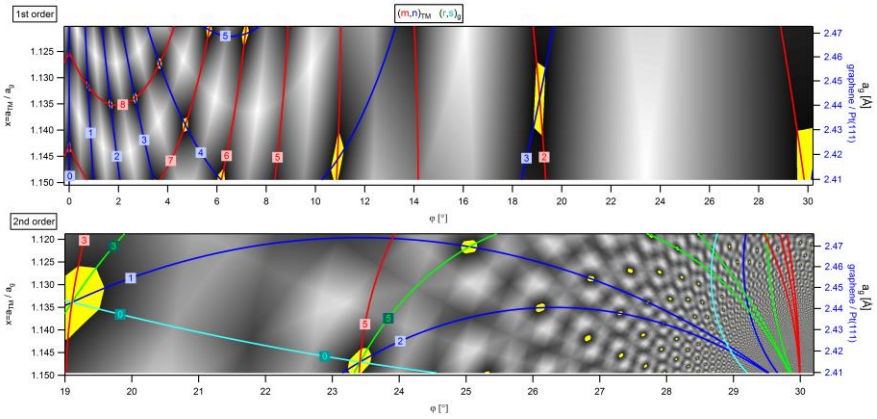

Figure 1: First and second order commensurability plots indicate possible unit cells for g-Pt(111). In particular, the indexing of the reported R19.2° and the R23.4° moiré pattern as a result of our analytical treatment is shown.

References:

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[2] K. Hermann, Journal of Physics: Condensed Matter **24** 314210 (2012).

[3] P. Zeller and S. Günther, New Journal of Physics **16,** 083028 (2014).