Crystallography of twisted bilayers moiré patterns
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Abstract
We show here that moiré patterns generated by 2D twisted homophase bilayers
rotated by 2δ, exhibit a quasiperiodic translational symmetry that is directly connected to the
so-called 0-lattice introduced long ago by W. Bollmann [1,2] in the geometrical description
of grain boundaries. Expressed in complex notations as an interference function between the
two layers, a typical moiré pattern μ(z) is the sum over the reciprocal lattice vectors of
products of a rapidly varying term of periods close to the ones of the lattice Λ of the layer,
multiplied by a slow varying term of periods twice the 0-lattice. The overall aspect of the
pattern is a quasiperiodic set of almost identical cells each centred on a node of the 0-
lattice. It will be demonstrated [3] that when coincidence lattices exist, for specific values of δ,
these are always subgroups of the 0-lattice of order η according to (p,q, n, m, k and r are
integers):
- rectangle system (p = |b|/|a| = v(p/q), γ =gcd(nq,mp): η = 4 n^2 q/γ if p>l for the rotation
  superposing the node (-n,m) to (n,m); η = 4 m^2 p/γ if p<1 for the rotation superposing the node
  (n,-m) to (n,m);
- square system: η = 2(n-m)^2/γ with γ =gcd(n+m,n-m) for the rotation superposing the node
  (m,n) to (n,m);
- hexagonal system: η = k^2 for the rotation superposing the node (k+2r, r+k) to (k+2r, r).

This shows that the moiré pattern has the exact periodicity of the coincidence lattice
only in the unique case of the hexagonal system for those specific coincidence rotations
superposing the nodes (1+2r,r+1) to (1+2r,r). In all other situations, the symmetry of the moiré
pattern, governed by the 0-lattice, is not to be confused with a possible coincidence lattice.

References

Figures

\[ O = \frac{i}{2 \sin \delta} e^{i\delta}(\Lambda + \tau), \quad \mu(z) = \sum_{\chi \in \Lambda} 2f_x e^{2i\pi (\cos \theta(x,z)+\varphi/2)} \cos 2\pi (\sin \theta(x).z - \varphi/2) \]

Figure 1: moiré pattern of an hexagonal bilayer rotated by 2δ = 9° decomposed into the sum
of products of fast and slow oscillating terms (the 0-lattice points are the red dots).