Dynamics and morphology of folds and wrinkles in graphene, h-BN and 2D talc

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We will report theoretical predictions [1] and experimental results [2,3] on the dynamics and morphology of folds and wrinkles in deposited 2D materials. First, we will present molecular dynamics simulations and analytical calculations of the dynamics of fold formation in laterally compressed 2D materials [1]. Our calculations lead to two main predictions. The first prediction is that fold formation starts with lattice instabilities in the form of extremely mobile soliton-like excitations that evolve into large, mobile folds. The second prediction is that the maximum curvature of a fold is proportional to the square root of the ratio between the layer bending modulus and the interlayer binding energy of the material. Therefore, fold morphology can be used to establish constraints between mechanical properties of 2D materials.
An experimental verification of fold mobility is found in the observation of the orientational ordering of wrinkles in annealed h-BN [2]. The wrinkles (which consist of folds) form a network of threefold junctions throughout the sample, the wrinkles being oriented along the armchair crystallographic directions (see figure). If the sample is quenched (instead of annealed) the wrinkles become orientationally disordered, indicating that ordering requires the motion of the wrinkles.
The second prediction - that fold morphology can be used to establish constraints between mechanical properties – is applied to the case of single- and few-layer talc. In this case, first-principle calculations show that the flexural rigidity of single layer talc should be more than thirty times larger than that of graphene [3]. This is consistent with the very large values of fold curvatures observed in this new 2D material.

References

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Figure - AFM characterization of h-BN flakes after annealing. (a) A 10nm-thick flake showing an orientationally ordered wrinkle pattern. The inset at the bottom left shows the FFT image of the flake topography. (b, c) Zoom-in AFM images acquired at the regions marked by white squares.