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Critical behavior of curvature localization in graphene[1] MRITYUNJAY KOTHARI, MOON-HYUN CHA, KYUNG-SUK KIM, Brown University — A multilayer graphene, when compressed, elastically buckles to a triangular crinkle shape even at the early stage of post bifurcation, with its maximum local slope change within a few degrees. Our DFT calculation shows that the graphene crinkle localizes and focuses surface curvature up to more than 10^{-1} nm^{-1} along a narrow ridge of approximately 1nm width, and nullifies it elsewhere. In contrast, Koiter analysis of multilayer buckling predicts a simple-mode supercritical bifurcation, and progressive weak curvature focusing up to at most 10^{-3} – 10^{-2} nm^{-1} in a width of tens of nm's. However, when we include flexo-electric effects explicitly in the classical model, we observe instantaneous localization of curvature, at the onset of bifurcation, down to 1 nm width with curvature focusing close to the DFT prediction. The localization produces curvatures up to three orders of magnitude higher than the maximum curvature of a single-layer graphene wrinkle with an equivalent amplitude. The computational and theoretical predictions are in good agreement with our experimental studies in which we also demonstrated aligning of charged molecules with crinkle surface charges of flexo-electric polarization.

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Kyung-Suk Kim
Brown University

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