Inserting defects into graphene: response by curvature and strain

"Bending Rules in Graphene Kirigami" by B.F. Grosso and E.J. Mele
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When exerting a force on a thin solid sheet, we often take it as granted that the sheet will deform by bending rather than by developing strain. This expectation stems from the sharp contrast between the sheet's bending and stretching moduli, which diverges as the sheet becomes thinner (at a rate proportional to the square of the sheet's thickness t). As was realized already by Euler more than two centuries ago, this dramatic difference between the two types of energetic costs is the essence of a fundamental instability: the buckling of solid plates and rods under compressive loads. However, sheets may be constrained in such a way that a strain-free deformation is impossible, for instance by confining a piece of paper in a small box. In such circumstances, a common assumption is that the unavoidable strain localizes in core zones – vertices and ridges – whose characteristic sizes vanish in the singular limit $t \to 0$ of an infinitely thin sheet [[5, 13, 15, 20]. The emergence of such "stress focusing" zones enables the rest of the sheet to remain strain-free, by deforming into *developable* pieces, such that the elastic energy in most of the sheet stems only from bending (except at the strained core zones). A basic example of a developable shape (*i.e.* with zero Gaussian curvature) is a cylindrical surface, and an example for a non-developable surface is a spherical cap (which has a positive, constant Gaussian curvature). The intimate link between developability and strain can be easily demonstrated by deforming a sheet of paper into these shapes. A cylindrical shape is obtained easily and smoothly, whereas deformation to a spherical cap typically leaves the paper with scars, indicating on the presence of domains with large strain.

In a recent paper [9], Grosso and Mele used atomistic simulations to study the response of graphene to an imposed dislocation in the lattice (generated by removing atoms from a finite strip in a flat graphene sheet and rejoining their neighbors, Fig. 1a,1b). The idea to study graphene's response to this type of defect (which the authors term "nano-kirigami") was motivated by a recent proposal for using kirigami – the art of folding and cutting paper – for an efficient construction of 3D faceted structures from inextensible planar lattices ([4] and see also a related commentary by M. Bowick [3]). However, what Grosso and Mele found in their simulations was very different from the faceted shapes described in [4]. The simulated graphene did not respond by decomposing into flat facets separated by sharp, stress-focusing creases (Fig.1c,1d); instead, the sheet adopted a smooth, curved shape (Fig. 1e,1f).

The surprise in this result can be understood by recalling previous studies that addressed the response of thin sheets to localized perturbations, *e.g.* by pushing a sheet of paper through a ring [5], or – in a work by Guven *et al.* which is closely related to Grosso and Mele's study – by creating an artificial "dislocation" at its center (by cutting out an angular sector, rotating and re-inserting it, and stitching all open cuts [10], see bottom right of Fig. 1). In those studies, the sheet is assumed to attain a developable shape, which is strain-free everywhere except at the vicinity of a localized defect and perhaps at some ridges separating flat or conical sections [21]. However, despite the apparent similarity between the shapes (Fig. 2 [10] and Fig. 1e,1f [9]), the deformation of the simulated graphene is **non-developable**; instead, the Gaussian curvature is found to vanish only upon (spatial) averaging, in a way that may arguably lower the strain, but is not being eliminated altogether. Thus, rather than focusing the unavoidable strain into small core zones, such that the energy is governed by the shape's curvature outside the core, the energetic cost of the deformed graphene sheet is governed both by strain and by the curvature of the shape. Motivated by their observation, Grosso and Mele proposed "nano-kirigami" rules for the shapes attained by graphene sheets in response to localized defects: Although the deformation generally consists of significant strain, only the bending part of the elastic energy is minimized, while only the average Gaussian curvature of the shape is required to vanish.

Is it possible that such "nano-kirigami" rules do characterize the ultimate response of very thin solid sheets to localized defects? Obviously, a graphene sheet cannot be made thinner, but one may increase its lateral size R (although a systematic numerical study may require a considerable computation time). Increasing the ratio between R and the atomic-scale thickness t (known as the von-Karman number $vk = (R/t)^2$), effectively increases the contrast between the characteristic energies of stretching and bending. Thus, when $R \gg t$, it seems natural to expect that the defected sheet will attain a developable shape, whose Gaussian curvature (and consequent strain) vanishes almost everywhere, rather than only on average. Yet, the Grosso-Mele's finding indicates on a surprisingly large transient regime (in the simulations of [9] $(R/t)^2 \sim 1000$), at which the deformed sheet is characterized by an intricate balance between curvature and strain, and cannot be assumed inextensible, as is often done.

There has been a considerable interest lately in classifying the distinct ways by which elastic sheets approach a strain-free (isometric) deformation in the singular limit of vanishing sheet's thickness. In addition to studies that addressed various types of developable (or piecewise developable) shapes [10, 12, 20], various groups generalized this idea to sheets whose strain-free state is associated with a non-flat metric ("incompatible elasticity") [7, 8, 11, 16], and to situations where the deformed sheets are subjected to weak tensile loads and reduce strain through non-developable

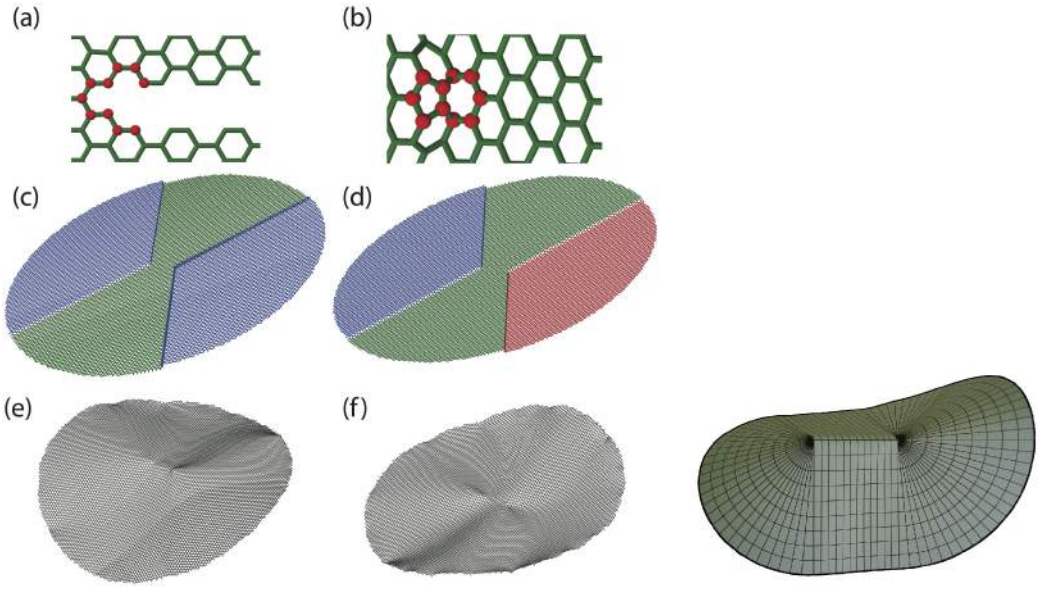

FIG. 1. Panels (a-f) are from Fig. 1 of [9] (Courtesy of E.J. Mele, see [9] for details). Panels (a,b) show the method for creating a dislocation in the graphene lattice by removing a row of atoms (a) and re-joining the two adjacent rows (b). The red sites mark the resulting dislocation which consists of complementary defects in the hexagonal lattice (a 5-ring and a 7-ring). Panels (c,d) show two possible modes of deformation (termed "up-up" and "up-down", respectively) to flat facets separated by sharp creases [4]. Panels (e,f) show the actual deformations in the simulated graphene sheet. The figure on the left (from Fig. 2 of [10], courtesy of J. Hanna) describes a developable deformation of a sheet, obtained upon cutting out an angular section, displacing slightly its apex, rotating and re-inserting it into the sheet (see [10] for details).

shapes riddled with wrinkles, folds [14, 19], or grain boundaries in crystalline sheets [1]. Other studies considered situations in which certain body forces or boundary constraints prevent the elimination of strain [2, 6, 17, 18]. The behavior found by Grosso and Mele, where the energy of the deformed sheet consists of comparable levels of strain and bending, is different from any of those mechanisms, demonstrating once again the surprisingly rich and complex phenomenology that springs from the deceptively simple energy of elastic sheets.

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