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Compressive failure of a carbon nano-tesseract: Sci-Fi inspired materials and the strength of thanos

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ABSTRACT

Inspired by the super-materials of science fiction ("sci-fi"), here we probe the stability and strength of a proposed all-carbon nano-tesseract or hypercube projected into 3D space, a so-called hypercubyne. The nanostructure is compared to other, similar carbon geometries of similar size, including a fullerene, a hypercubane, and a pentatope. The hypercube configurations provide high compressive strength and elastic toughness with an open lattice structure. For the all-carbon hypercubyne, initial failure is characterized by a buckling instability. Using the ultimate strength of hypercubyne as a basis, we proceed to predict the lower bound of the strength of the supervillain Thanos, who has been depicted destroying the Tesseract in the Marvel Cinematic Universe. Thanos has a minimum grip strength of over 40,000 tons, which is approximately 750,000 times that of a typical man. While such comic-inspired analysis is whimsical by design, the study sheds light into the behavior of future exotic carbon constructs and geometries, and illustrates the potential field of "sci-fi" inspired materials.

1. Introduction

While science progression is ultimately rooted in reality (and governed by physical laws), there is no global constraint imposed on source of inspiration or one's imagination [1]. Indeed, creativity does not play by physical rules [2]. As a direct result, some of the most creative and inspiring ideas may arise from science fiction (or "sci fi") — and in this particular case, the superhero universe. Indeed, exotic materials play a unique role in superhero lore [3], particularly when feats of extreme strength, toughness, and resilience are necessary — *i.e.*, extreme mechanics. Comic aficionados may refer to the *adamantium* claws of Wolverine (not to be confused, of course, with adamantane [4]), or the *vibranium* shield of Captain America (from Wakanda, of course). The defining quality of adamantium is its practical indestructibility. For vibranium, absorbing sound waves and kinetic energy makes this metal stronger. Such properties are quite useful when fending off supervillains, but difficult to model in practice.

Here, rather than exotic *materials* per se, we consider exotic *geometry* of materials. Recent advances in materials science have enabled fabrication of structures with almost arbitrary three-dimensional (3D) geometries, across length scales, made out of a wide range of materials [5]. At the same time, it is recognized that structural configuration/architecture/geometry may be just as important to emergent material properties as the base components and elements themselves [6–9]. This particular work is motivated by the appearance (or more specifically, the destruction) of the Tesseract in *Marvel Cinematic Universe* (MCU). In geometry, a tesseract is the four-dimensional analogue of the cube — a tesseract is to the cube as the cube is to the square — *e.g.*, take a cube and extrude it into a fourth spatial dimension. Clearly, this cannot be physically accomplished (with current technology). However, a 3D representation of a tesseract is commonly represented as a *cube-within-a-cube* construct, as depicted in Fig. 1(a). In the MCU, *the Tesseract* is a crystalline cube-shaped containment vessel one of the six Infinity Stones that predate the universe and possesses unlimited energy, Fig. 1(b). To harness the power of an Infinity Stone, the hypercube itself must be made of an extremely strong material. Since the cube is known as the Tesseract, it may also be prudent to assume the base molecule could potentially be a similar hypercube-geometry, realized in three-dimensions. Perhaps the creators of the Tesseract were proponents of symmetry and hierarchies — key concepts of materials design [10–14]. Here, we propose a tesseract-*like* 3D molecule composed of all carbon atoms (Fig. 1(c)).

Such multi-dimensional geometries are well-defined mathematically, and the hypercube/tesseract is one of the six known 4D regular polytopes (4-polytopes). The 4-polytopes are the four-dimensional analogs of the regular polyhedra in three dimensions and the regular polygons in two dimensions [15,16]. Due to the interest in carbon-allotropes and carbon-based macromolecular

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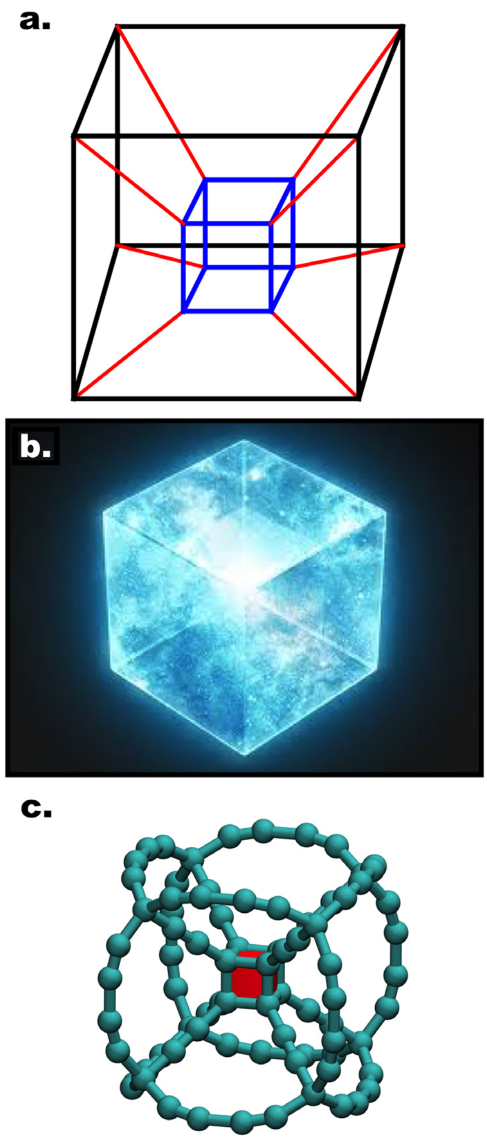

Fig. 1. Schematics of (a) 3D representation of a tesseract or hypercube, depicted by a cube-within-a-cube geometry; (b) screenshot of *the* Tesseract from the Marvel Cinematic University (MCU), vessel of one of the six Infinity Stones, material unknown (image is a screenshot of a copyrighted film; depicted under the fair use provision of United States copyright law); (c) molecular carbon-based tesseract analog, denoted hypercubyne.

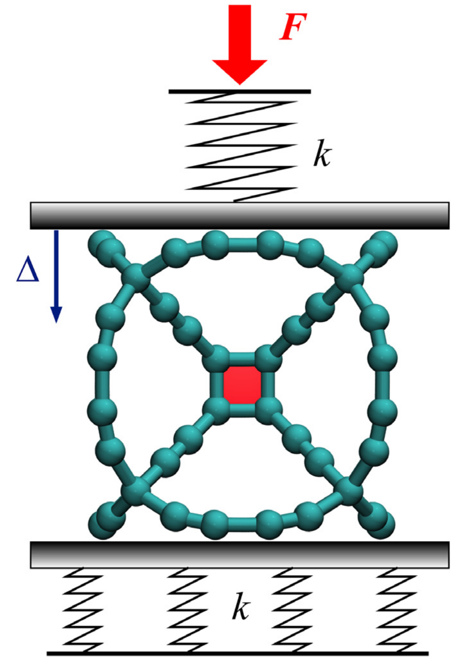

Fig. 3. Schematic of compression test. Molecules are compressed between two elastic surfaces represented by planes with harmonic springs of stiffness k. One surface is fixed (lower), while the other (upper) is displaced, Δ, at a constant rate. The spring force, F, necessary for deformation is recorded.

chemistry, it is likely that if such molecular geometries are to be accessible synthetically in the future, a carbon-based platform would be rational [17]. In fact, a carbon-based tesseract geometry — so-called *hypercubane* —has previously been proposed and investigated *via* DFT and tight-binding methods [18–20]. Moreover, prior studies have also explored the potential for expanded cubane *via* acetylenic linkages [21,22]. Here, we propose and model an all-carbon acetylenic-based tesseract we label hypercubyne. For stability comparisons, we also model: the previously proposed hypercubane; an all-carbon tetrahedra-based 4-polytope, also called a *pentatope* (similar to an expanded carbon tetrahedrane [23]), and; a C_{96} fullerene (see Fig. 2). All structures have approximately the same dimension (on the order of 0.8 nm in both height and width). We note that other carbon constructs of the remaining four theoretical 4-polytopes (the 4-orthoplex, octaplex, dodecaplex and tetraplex) were not stable *via* preliminary modeling. Our primary goal is to quantify the theoretical strength of the hypercubyne, to predict the ultimate strength of the MCU Tesseract (as well as to probe the benefits and penalties of such exotic geometries).

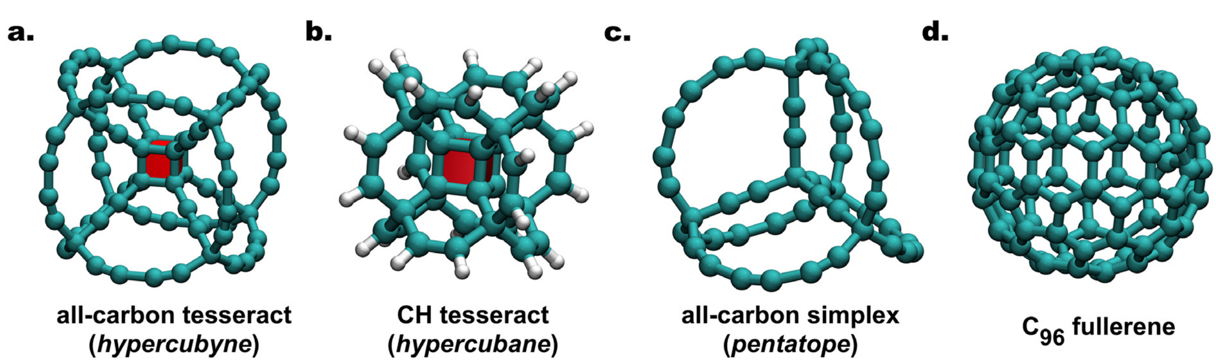

Fig. 2. Molecular structures of modeled geometries, including (a) hypercubyne (all-carbon), (b) hypercubane (carbon + hydrogen), (c) an all-carbon tetrahedral-based 4-polytope, a.k.a. a simplex or pentatope, and (d) a C_{96} fullerene, the only readily available molecule with similar size and carbon composition.