A Theoretical Consideration of the Ballistic Response of Continuous Graphene Membranes

Eric D. Wetzel*, Radhakrishnan Balu, and Todd D. Beaudet

U.S. Army Research Laboratory

Weapons and Materials Research Directorate and Computational and Information Sciences

Directorate

Aberdeen Proving Ground, MD 21005

*eric.d.wetzel2.civ@mail.mil, 410-306-0851

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Abstract

The remarkable properties of graphene, including unusually high mechanical strength and stiffness, have been well-documented. In this paper, we combine an analytical solution for ballistic impact into a thin isotropic membrane, with *ab initio* density functional theory calculations for graphene under uniaxial tension, to predict the penetration resistance of multi-layer graphene membranes. The calculations show that continuous graphene membranes could enable ballistic barriers of extraordinary performance, enabling resistance to penetration at masses up to 100× lighter than existing state-of-the-art barrier materials. The very high elastic wave speed and strain energy to failure are the major drivers of this increase in performance. However, the in-plane mechanical isotropy of graphene, as compared to conventional orthotropic

woven textiles, also contributes significantly to the efficiency of graphene as a barrier material. This result suggests that, for barrier applications, isotropic membranes composed of covalently bonded two-dimensional molecular networks could provide distinct advantages over fiber-based textiles derived from linear polymers.

Keywords: graphene, ballistics, armor, impact, textiles

1. Background

Ballistic barriers for body armor, turbine blade confinement, or space debris shields are important technological structures for which the common goal is to resist penetration from a high velocity projectile, usually while minimizing weight and/or bulk. In many cases, textiles woven from high performance yarns such as aramids (for example DuPont™ Kevlar® fibers) or ultrahigh molecular weight polyethylene (UHMWPE) (for example Honeywell Spectra® fibers) are major components in these barrier materials, primarily because they have among the highest density-normalized stiffness and strength of commercially available materials. In other specialty armors, not of interest to the present discussion, hard ceramic strike faces are also included to break up the projectile and consume energy during the comminuted flow.

The recent emergence of graphene as a material of extraordinary strength and stiffness [1, 2] suggests that it may provide unprecedented capabilities as a ballistic barrier material. Indeed, recent experimental results [3] are consistent with this expectation. In this paper, a theoretical estimation of the potential performance of graphene as a ballistic barrier is presented. First, analytical impact theory is used to establish scaling parameters for ballistic penetration response, and highlight the fundamental difference in response for isotropic membranes such as graphene

versus orthotropic, woven textiles. The in-plane uniaxial stress response for a graphene membrane is then generated via *ab initio* density functional theory, and applied to estimate ballistic scaling parameters for graphene and predict the behavior of graphene relative to conventional ballistic barrier materials. In addition, to eliminate some of the uncertainty associated with estimating graphene performance using a linear elastic, small deformation theory, predictions are also provided for a "sub-graphene" notional material with elastic properties identical to graphene, but exhibiting small strains to failure.

2. Isotropic versus Orthotropic Ballistic Barriers

The mechanics of ballistic impact are complex, but the case of normal impact into a thin isotropic membrane can nominally be described as follows [4]. Upon initial contact, a momentum exchange between the projectile and the barrier leads to a rapid partial deceleration of the projectile. A radial in-plane tensile wave then emanates from the impact point at a speed comparable to the elastic wave speed in the material, pulling barrier material towards the projectile. Simultaneously, the projectile is travelling normal to the barrier, creating a transverse deformation cone which continuously decelerates the projectile. Radial tensile loads build in the vicinity of the projectile and, if local stresses exceed failure conditions for the barrier, perforation occurs. If, instead, the projectile is completely decelerated prior to penetration, the projectile is stopped. In this model of barrier impact, the primary loads on the barrier are in-plane tension and, therefore, it is these properties that are the major determinant of ballistic response.

The ballistic response of most barriers is probabilistic; that is, a given set of ballistic conditions (consistent armor composition, armor areal density, mechanical boundary conditions, and projectile characteristics) can result in either a penetrative or non-penetrative event. The

probability of penetration tends to increase as impact velocity increases, with penetration being highly unlikely at very low velocities and nearly certain to occur at very high velocities. The first-order parameter that is typically measured and reported to represent the characteristic ballistic limit of a particular barrier is the velocity at which the probability of penetration is 50%, referred to as the V_{50} velocity [5]. For analysis purposes, this velocity represents, on average, the velocity at which the projectile is just barely stopped by the barrier. Said differently, the V_{50} represents, in an average sense, the condition where the initial kinetic energy of the projectile is exactly balanced by the available deformation and failure energy within the interacting volume of the barrier material.

Using dimensional analysis and empirical fitting to experimental ballistic data, Cunniff [6] showed that the limiting penetration velocity for a homogeneous (all layers composed of identical materials) textile barrier scales with the material parameter

$$\Lambda_y = (\bar{U}_y \cdot c_y)^{1/3} \quad (1)$$

where $\bar{U}_y$ is the mass-normalized tensile strain energy to failure (J/g) of the yarns in the textile, and c_y is the longitudinal elastic wavespeed in the yarns, given by

$$c_y = \sqrt{\frac{E_y}{\rho}} \quad (2)$$

Here, E_y is the longitudinal elastic modulus of the yarns. Using similar scaling arguments, Cunniff also hypothesized that the performance of a barrier material should be driven by the mass ratio parameter Γ , defined as

$$\Gamma = \Theta \frac{\rho h}{m_p / A_p} \quad (3)$$

where m_p is the projectile mass, A_p is the projectile presented area, ρ is the barrier density, and h is the barrier thickness. Θ is a factor to account for effects such as obliquity and projectile blunting, with a typical value of 1.5-1.8 required for good agreement between theory and experimental data [4]. To demonstrate the utility of these scaling parameters, Cunniff showed that ballistic data for a variety of aramid and nylon textiles and textile composites could be collapsed to a single empirical function for V_{50}/Λ_y as a function of Γ . The same empirical function tended to overpredict the ballistic performance for UHMWPE textiles and composites reinforced with UHMWPE, carbon fiber, and glass fiber.

Following this scaling study, Porwal and Phoenix [4] derived an analytical solution for the impact of an infinite, linear elastic, thin isotropic membrane by a cylindrical projectile. The derivation assumes a self-similar deformation cone shape, neglects Poisson's ratio effects (resulting in very small errors for materials with Poisson's ratio less than 0.3, a condition predicted to be met for graphene by most simulations to date [7]), and eliminates many higher order terms (insignificant in value for most practical ballistic conditions) in order to produce a closed-form analytical solution for the strain and displacement history of the impacted membrane. This analysis predicts that the membrane limiting velocity (V_{50}^{membrane}) should be proportional to

$$V_{50}^{\text{membrane}} = \sqrt{2}(1 + \Gamma)c_m(\varepsilon_m / K_m)^{3/4} \quad (4)$$

where c_m is the linear wavespeed in the membrane, ε_m is the maximum strain to failure in the membrane, K_m is a function that depends on both Γ and ε_m . Since the solution is derived for a linear elastic material, this relation can be recast as

$$\frac{V_{50}^{\text{membrane}}}{\Lambda_m} = 2^{5/6}(1 + \Gamma)\varepsilon_m^{1/12}K_m^{-3/4} \quad (5)$$

where

$$\Lambda_m = \left(\frac{\sigma_m \varepsilon_m}{2\rho} \cdot c_m \right)^{1/3} = \left(\frac{E_m \varepsilon_m^2}{2\rho} \cdot c_m \right)^{1/3} = c_m \left(\frac{\varepsilon_m^2}{2} \right)^{1/3} \quad (6)$$

and E_m and σ_m are the tensile elastic modulus and failure stress in the membrane, respectively.

Equation (5) shows that Λ_m alone is not rigorously sufficient to capture the effects of material properties on V_{50} scaling, since ε_m appears on the right-hand-side (RHS) of this equation

(including within the K_m function). However, it can be shown that Λ_m varies more strongly with ε_m compared to the variation of the RHS of Eqn. (5) with respect to ε_m ; for example, for a value of $\Gamma=0.2$ (representative of a 1 gr steel projectile impacting a typical 30-layer Kevlar target) as ε_m varies from 0.01 to 0.2, Λ_m varies by a factor of 7 while the RHS of Eqn. (5) varies only by a factor of 1.9. Therefore Porwal and Phoenix argue that it is reasonable, although not exact, to use Λ_m as a material scaling factor for the prediction of V_{50}^{membrane} performance.

To apply this solution for isotropic membranes to plain-woven (orthogonal yarn) textiles, Porwal and Phoenix modify their solution by accounting for the fact that only half of the yarns in the fabric contribute to loading in each principal direction. The final solution for predicted ballistic limit for a textile (V_{50}^{textile}) is

$$\frac{V_{50}^{\text{textile}}}{\Lambda_y} = 2^{1/3} (1 + \Gamma) \varepsilon_y^{1/12} K_y^{-3/4} \quad (7)$$

where Λ_y and K_y are functions identical to Λ_m and K_m , but are calculated using elastic yarn properties E_y , ε_y (strain to failure), and σ_y (failure stress). Comparing this equation to the relationship for the V_{50} of an isotropic elastic membrane (Eqn. 5), under conditions of identical yarn and membrane tensile properties we find that

$$V_{50}^{\text{membrane}} = \sqrt{2} \cdot V_{50}^{\text{textile}} \quad (8)$$

This relationship provides our first crucial result: comparing an isotropic membrane to a woven textile of identical mass, if the textile yarns have identical tensile properties to the isotropic membrane, the critical penetration velocity for the membrane will be approximately 40% higher than the woven textile. Despite this advantage, conventional isotropic membranes, such as metal foils and polymer films with randomly oriented linear polymers, do not have sufficient density-normalized mechanical strength and stiffness to compete with state-of-the-art fibers composed of highly aligned linear polymers. The emergence of graphene and other two-dimensional polymers presents an opportunity to reconsider isotropic membranes.

3. Mechanical Response of Graphene

To evaluate the potential of graphene as a ballistic barrier, its representative mechanical properties are required. We can limit our consideration to uniaxial tension, as the tensile radial stresses during ballistic impact far exceed the slightly compressive circumferential (hoop) stresses (which, in practicality, are most likely accommodated via out-of-plane buckling rather than true compression) [4]. Prior experimental [1] and computational studies [8, 9] have shown that graphene at high strains obeys a non-linear elastic response which, under uniaxial tension, can be expressed phenomenologically as

$$\sigma = E_m \varepsilon + D_m \varepsilon^2 \quad (9)$$

where σ is the tensile stress (first Piola-Kirchhoff stress), ε is the tensile strain (change in length normalized by original length), E_m is the linear Young's modulus, and D_m is the non-linear elastic modulus. Since a graphene monolayer does not have a well-defined thickness, stress and moduli are expressed as two-dimensional values with units of N/m. For a negative D_m value, the

maximum stress occurs at $\sigma_m = -E_m^2/(4D_m)$ and $\varepsilon_m = -E_m/(2D_m)$. Integrating Eqn. (9) with respect to strain gives the strain energy density U of the material during uniaxial tension:

$$U = \frac{1}{2} E_m \varepsilon^2 + \frac{1}{3} D_m \varepsilon^3 \quad . \quad (10)$$

The strain energy at failure ($\varepsilon = \varepsilon_m$) is therefore $U_m = 4\sigma_m^2/(3E_m)$ where, if two-dimensional moduli are used for E_m and D_m , then U_m is an area-normalized energy (J/m²).

Values of E_m and D_m for graphene have been reported, primarily calculated via molecular dynamics [8-10] but also supported by at least one experimental data set [1] (Table 1). We complement this data by performing *ab initio* Kohn-Sham density functional theory (DFT) based computations using the Gaussian and plane wave-method code QUICKSTEP as implemented in CP2K [11]. The calculations use the generalized gradient approximation (GGA) exchange-correlation functional BLYP due to Becke [12] and Lee, Yang, Parr [13]. The 1s² carbon core states are accounted for by Goedecker, Teter, and Hutter (GTH) pseudopotential [14, 15] optimized for BLYP by Krack [16]. A Gaussian basis set with double-zeta and valence polarization functions fit for BLYP/GTH was used to describe the single-body orbitals. The density was described by plane wave basis with 350 Ry cutoff. We treat the Gamma point of the Brillouin zone using a super cell (4×4×1 unit cell) with 32 atoms and graphene layers spaced by 15 Å. Dispersion interactions are accounted for using the DFT-D method with D3 parameterization as implemented in CP2K [17, 18]. Total energies, energy gradients and lateral stresses were converged to 1.0×10⁻⁶ Hartree, 4.5×10⁻⁴ Hartree/Bohr, and 100 bar respectively throughout. Calculations were performed for uniaxial tension in both the zigzag (second nearest neighbor) and armchair (nearest neighbor) directions [8], at strain increments of 0.5% up to peak strains of 27% and 25% strain, respectively. The CP2K framework accepts finite-strain initial

conditions, therefore the prediction of uniaxial stress response required the use of an external script. Using the stress-free equilibrium structure as an initial condition, a uniaxial strain of 0.5% was applied in the direction of interest. The lateral strain was then relaxed slightly, and a new solution calculated, resulting in reduced lateral stress. This process of transverse relaxation was performed iteratively via the external script, until the lateral stress was reduced to zero within the 100 bar convergence limit. This process was repeated in increments of 0.5% strain to generate the overall material response curves in the armchair and zigzag directions. The resulting lattice energy, normalized by initial unit cell area, and stress responses are shown in Fig. 1. The energy data was fitted according to Eqn. (10) in both armchair and zigzag directions simultaneously, producing a single E_m value and separate armchair and zigzag D_m values. The results are given in Table 1, with a single D_m reported as the orientationally averaged value (equal to the simple average of zigzag and armchair directions [8]). Values of $E_m = 329$ N/m and $D_m = -691$ N/m, calculated as the average of all reported values from Table 1, are used for subsequent quantitative estimations of graphene mechanical response.

The two-dimensional (areal) density of monolayer graphene can be estimated to be 7.42×10^{-7} kg/m², based on hexagonal symmetry and a bond length of 0.144 nm (the equilibrium configuration from CP2K, very close to the value of 0.142 nm reported for single crystal graphite [19]). Combining this areal density with the elastic modulus from Table 1, Eqn. (2) gives a low-strain wavespeed for graphene of 21.0 km/s. Normalizing the per-area energy to failure from Table 1 by the areal density gives a mass-normalized energy to failure of 8350 J/g.

4. Theoretical Ballistic Predictions for Graphene

Using the average wavespeed and deformation energy at failure from Table 1, the ballistic parameter of Eqn. (6) has a value of $\Lambda_m=5600$ m/s for graphene. This value is compared to other engineering materials in Table 2. Materials above the dashed line are textiles, while materials below the dashed line are isotropic membranes. Also tabulated are ballistic limits normalized by the ballistic limit of a Kevlar membrane of comparable mass. These ratios are calculated by assuming that V_{50} is proportional to Λ , and that isotropic membranes will have a ballistic limit that is higher than woven textiles of comparable mechanical properties by a factor of $\sqrt{2}$ per Eqn. (8). The results show that most engineering textiles are expected to provide comparable ballistic response, with emerging materials such as spider silk (the value given is the highest strain energy density reported for spider silk, based on a unique species [20]) and carbon nanotube (CNT)-based yarns [22] providing opportunities for more significant performance enhancements. Conventional metallic and polymer isotropic membranes perform similar to, or worse than, Kevlar textile membranes. In comparison, graphene, with isotropic properties and relatively high wave speed and strain energy density, is expected to produce a remarkable 12× increase in ballistic limit.

Equation (5) was derived for a linear elastic material at low strains. The application of this theory to graphene, with non-linear elastic behavior and high strain-to-failure, results in predictions with considerable uncertainty. Therefore it is instructive to also consider a "sub-graphene" membrane, with an E_m equal to graphene but assumed to exhibit linear elastic behavior to a failure strain of only 3.3% (matched to Kevlar), given in Table 2. The simulations confirm that graphene exhibits linear response at low strains (Fig. 1), and by matching the peak strain to that of Kevlar the weaker strain dependencies in the RHS of Eqn. (5) are rigorously

eliminated from the V_{50} ratio calculation. Furthermore, since it may not be possible to produce single-crystal graphene at engineering scale, the sub-graphene can also represent an imperfect graphene membrane whose strength is compromised by flaws such as vacancies and grain boundaries. In spite of the drastically reduced strain to failure, this material is still expected to possess a V_{50} value over $3\times$ higher than a Kevlar barrier of comparable mass.

It is also critical to determine the mass of graphene membrane necessary to match the ballistic limit of a given Kevlar barrier, i.e. the potential weight savings. The barrier areal density is captured by the barrier-to-projectile mass ratio Γ , but since Γ is also embedded within K one can not easily separate mass effects from Eqns. (5) and (7). As a simple approximation, the projectile kinetic energy scales with the square of its velocity, therefore the square of the V_{50} ratio given in Table 2 is a crude metric of the relative failure energy density of the barrier, and one would therefore expect that

$$\frac{\Gamma_m}{\Gamma_{\text{Kevlar}}} \approx \frac{1}{2} \left(\frac{\Lambda_{\text{Kevlar}}}{\Lambda_m} \right)^2 \quad (11)$$

where the factor of $1/2$ is necessary per Eqn. (8) since we are comparing a woven textile to an isotropic membrane. This relation predicts that a sub-graphene membrane would be roughly 8% the mass of a Kevlar barrier with comparable V_{50} , while a graphene membrane would be approximately 0.7% of the Kevlar barrier mass. To provide higher confidence in this trend, we implement the full solutions of Eqn. (5) for sub-graphene and graphene, and Eqn. (7) for Kevlar (see [4] for full expansion of K in terms of ε and Γ). Calculations are performed using the properties of Table 2, over a range of Γ for each material that gives V_{50} values from 100-1000 m/s (typical of barrier applications such as body armor) (Fig. 2a). This data is then used to calculate mass ratios for graphene and sub-graphene relative to Kevlar at each V_{50} . Interestingly,

these mass ratios show only a weak dependence on Γ (via K in Eqns. (5) and (7)); the average mass ratio values are 12% for sub-graphene and 0.5% for graphene over the full range of Γ .

Empirically we find that the analytical data is well-fit (Fig. 2) by the relation

$$\frac{V_{50}}{\Lambda} \approx \frac{1}{\alpha} \cdot 2^{13/4} \epsilon^{1/3} \Gamma^{3/5} \quad (12)$$

where $\alpha = 1$ for isotropic membranes and $\alpha = \sqrt{2}$ for textiles per Eqn. (8). Using this empirical relationship, the mass ratio is then predicted to be

$$\frac{\Gamma_m}{\Gamma_{\text{Kevlar}}} \approx \frac{1}{2^{5/6}} \left(\frac{\Lambda_{\text{Kevlar}}}{\Lambda_m} \right)^{5/3} \left(\frac{\epsilon_{\text{Kevlar}}}{\epsilon_m} \right)^{5/9} \quad (13)$$

which gives mass ratios (relative to Kevlar) of 12% for sub-graphene and 0.6% for graphene.

Taken together, these calculations predict that a sub-graphene barrier would be roughly 10× lighter than a comparable Kevlar barrier, while a graphene barrier would be over 100× lighter.

5. Discussion and Conclusions

These theoretical predictions have a number of caveats. First, as mentioned above, the ballistic penetration theory was derived under the assumption of low strains and linear elasticity, while the full graphene response is non-linear elastic and fails at relatively high strains; improved predictions require a more general theory that is not presently available. (However, it should also be noted that the basic material parameters of the model - wavespeed and mass-normalized energy to failure - are reasonably well-characterized for graphene, and therefore the basic scaling arguments presented herein should hold to order-of-magnitude accuracy.) Secondly, the theory assumes that membrane failure is dominated by in-plane tension, and that other local loads such as transverse compression and shear do not trigger premature failure. This assumption often holds true for high performance fibers like Kevlar and UHMWPE that are unusually adept at

maintaining tensile strength in the presence of transverse loading [24-26]. Little is known about graphene failure under multi-axial loading. Similarly, the model does not take into consideration flaw effects, grain boundaries, and crack growth. Simulations of failure in graphene predict significant strength reductions due to grain boundaries [27-29] and atomic vacancies [30]. While experiments to directly measure fracture toughness have not achieved consensus [31-32], other experiments have demonstrated that the strength and stiffness of polycrystalline graphene films as measured via center-loading of a suspended membrane can be comparable to values for single crystal graphene if best-practices synthesis and transfer steps are implemented [3]. Finally, this analysis derives mechanical properties from single layer graphene simulations, while the ballistic predictions are meant to represent many layers of graphene loaded simultaneously. Simulations and experiments are needed to better understand how loads are shared between graphene layers during ballistic impact. We also note that the theory requires membrane behavior with negligible bending stiffness, while millions of graphene layers (e.g. crystalline graphite) behaves like a rigid plate. A flexible graphene ballistic barrier would need to be composed of many thin, individual graphitic sub-membranes, each composed of hundreds or perhaps thousands of layers of graphene but mechanically distinct so that the assembly remains flexible, similar in form to a stack of high strength films or foils.

Considering these caveats, it is useful to compare our theoretical predictions relative to very recent "microballistic" experiments on many-layer graphene (MLG) membranes [3]. In these experiments, edge-supported, unbacked HOPG membranes of 10-100 nm thickness (30-300 layers of graphene) are penetrated by 3.7- μm -diameter glass spheres with an impact velocity of 600 or 900 m/s. The results show that the per-mass energy absorbed by the MLG membranes is 5-10 $\times$ higher than those of gold films and polymer films. Furthermore, using scaling

arguments to compare these results to macroscopic ballistic data, the energy absorption in the MLG membranes is approximately 50% higher than that of Kevlar composite membranes. Although this improved performance relative to Kevlar quite impressively demonstrates graphene's efficiency as a ballistic barrier, the present theory predicts that the energy absorption has the potential to be 10-100× higher than Kevlar. Significant crack propagation away from the impact site could be an indication that a more detailed treatment of flaw effects and fracture mechanics is needed to explain the experimental data set relative to theory. It should also be noted that the theory is derived for an infinitely large membrane, whereas the experimental membranes are finite in size. Considering the high in-plane wave speed for graphene, it is likely that significant stress wave reflections and interactions exist in the experiments, which could generate stress concentrations that trigger premature failure.

We also note a number of secondary advantages of isotropic membranes compared to woven textiles. The strength of yarns can be significantly degraded (up to 20%) during the weaving process [33], so the final barrier strength of a textile may lag behind its theoretical potential. Isotropic membranes, in contrast, could be stacked to form ballistic barrier, avoiding the mechanical degradation associated with weaving. Yarns are not closely held together, therefore "windowing" processes may occur that allow sharp-tipped projectiles or stabbing threats to push aside yarns and penetrate without significant fiber failure [34]; such a mechanism would not be operable in an isotropic membrane. Woven textiles also possess crimp (yarn undulations) that straighten during impact, which can exaggerate the transverse deflection cone exhibited by the barrier; planar membranes have no crimp, and therefore should be capable of stopping projectiles at much lower backface deflection values, reducing secondary damage to supporting materials or minimizing blunt trauma to a body armor wearer. Roylance et al. [35]

also speculated that yarn cross-overs trigger local longitudinal stress wave reflections that can induce premature barrier failure.

In summary, we have shown that multi-layer stacks of continuous graphene membrane could provide a revolutionary advance in ballistic barriers. In fact, graphene is only one example of the broad field of two-dimensional polymers [36-44], many of which would be expected to exhibit nominally isotropic high strength and stiffness. Other two-dimensional materials such as BN [45] and MoS₂ [46] are also predicted to provide excellent in-plane mechanical properties although at values that are somewhat lower than graphene. The major challenge is to develop techniques to fabricate these materials at sufficient scale for technological use. We note that, even if the 100× mass savings for graphene versus Kevlar is realized, over 50,000 layers of graphene would be needed to create a barrier comparable to a 4 kg/m² Kevlar body armor. The continuous nature of the membrane is key, therefore we would expect that using finite graphene flakes (smaller in size than the projectile diameter, e.g. 10 mm or smaller) as reinforcement in a polymer will not provide the necessary performance. Scalable techniques for growing large sheets, or stitching together finite sheets, at a massive scale are needed. One should also consider that carbon nanotube yarns can, in theory, produce equivalent mechanical properties to graphene. However, the theoretical arguments of the present study suggest that a continuous graphene membrane would considerably outperform (40% higher V_{50}) an equivalent mass carbon nanotube textile.

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Tables

Table 1. Comparison of experimental measurement [1] and computational simulations [8 - 10] of the linear and non-linear elastic properties of graphene. Elastic constants for Liu et al. are based on a fit of Eqn. (10) to their published data points.

Source	E_m (N/m)	D_m (N/m)	ϵ_m (%)	σ_m (N/m)	c_m (km/s)	U_m (J/m ²)	$\bar{U}_m$ (J/g)
[1] (Exp.)	340	-690	25	41.9	21.4	6.88	9270
[8] (DFT)	312	-583	27	41.7	20.5	7.44	10000
[9] (DFT)	320	-685	23	37.4	20.8	5.82	7840
[9] (MD)	320	-615	26	41.6	20.8	7.22	9730
[10] (DFT)	341	-771	22	37.7	21.4	5.56	7490
this study (DFT)	340	-805	21	35.8	21.4	5.04	6790
Average	329	-691	24	39.1	21.0	6.19	8350

Table 2. Comparison of expected ballistic performance of various materials. Materials above the dashed line are textiles, with mechanical properties for fibers / yarns / tows reported.

Materials below the dashed line are isotropic membranes. V_{50} ratios in the last column are calculated by normalizing each material's Λ by the Λ for Kevlar, and multiplying by $\sqrt{2}$ for the isotropic membranes. For most materials, strain energy density is estimated from strength and strain-to-failure data by assuming linear elastic behavior. For the CNT yarn, strain energy is directly reported by the source. Graphene wave speed and strain energy density are from Table 1, with three-dimensional stress and modulus values calculated for comparison purposes by assuming a graphitic layer spacing of 0.335 nm [19] Sub-graphene is treated as a linear elastic isotropic membrane with a modulus equal to that of graphene, and a strain to failure of 3.3%.

Material	Source	Density (g/cc)	Young's modulus (GPa)	Tensile strength (GPa)	Strain to failure (%)	Wave speed (km/s)	Strain energy density (J/g)	Λ_y or Λ_m (m/s)	$V_{50} /$ $V_{50, \text{Kevlar}}$ (m/s)
Kevlar 129 (840d aramid yarn)	a	1.44	96	3.38	3.3	8.2	38.7	681	1.00
Dyneema SK-76 (400d UHMWPE yarn)	a	0.98	88	2.62	3.6	9.5	48.1	770	1.13
Zylon (500d PBO yarn)	a	1.54	180	5.8	3.5	10.8	65.9	893	1.31
Nylon (800d polyamide yarn)	a	1.2	5	1	20	2.0	83.3	554	0.81
carbon fiber (7200d PAN-based tow)	a	1.8	234	4.83	2	11.4	26.8	674	0.99
spider silk (<i>Caerostris darwini</i>)	[20, 21]	1.3	11.5	1.65	50	3.0	317	981	1.44
CNT yarn	[22]	0.9	357	8.8	2.5	19.9	121	1340	1.97
aluminum alloy 5083	b	2.66	70.3	0.317	16	5.1	9.5	366	0.76
titanium alloy Ti-6-4	b	4.43	114	1.86	14	5.1	29.4	530	1.10
AISI 4340 steel, oil-quenched	b	7.85	196	1.86	12	5.0	14.2	414	0.86
polycarbonate	[23]	1.2	2.38	0.066	110	1.4	30.3	349	0.72
graphene	Table 1	2.21	981	117	24	21.0	8350	5600	11.6
sub-graphene		2.21	981	32	3.3	21.0	241	1720	3.57

^amanufacturer data ^basm.matweb.com

Figures

Figure 1: Computational predictions of (a) lattice energy versus strain and (b) two-dimensional stress versus strain for graphene under uniaxial extension along zigzag and armchair directions.

For clarity, every-other data point from the simulation data set is shown.

Figure 2. (a) Analytical (Eqns. 5 and 7) and empirical (Eqn. 12) relationships between V_{50} and Γ for Kevlar, sub-graphene, and graphene. (b) Scaled V_{50} data as a function of Γ .