Forging a Low-Carbon Future With CNT-Reinforced Steel

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ABSTRACT

Steel productions worldwide amount to approximately 7 % of the global CO_2 emission bsed on the data from International Energy Agency (IEA). Steel is an alloy of iron and carbon, engineered for enhanced strength. During the last 70 years, with advancements in its development, it has changed the way we live our lives and has shaped modern life. From structural elements to critical and strategic applications, steel has played a significant role. Here, I will discuss the significance of CNTs in optimization of steel. I further argue that these breakthroughs have the potential to provide solutions to climate and engineering challenges. Examples range from sustainable urban structures, to design of components which can endure extreme plasma temperatures in future fusion reactors or space missions necessary to understand the Earth's climate and history. Discussing the physics of CNTs in detail, CNT-reinforced steel will be discussed through the lens of climate engineering and its potential to reduce the need for steel production itself. Facilitating the creation of lightweight, high-strength materials is another application. I argue that such innovations can significantly reduce CO_2 emissions in aviation and other industries as well, paving the way for a low-co_2 future, contributing to solutions for the climate crisis.

Keywords: Materials Design, Steel, Carbon Nanotubes, Climate Change

CONTENTS

1 INTRODUCTION

Steel production, a critical industry with significant impact on the global economy, is also a playground for condensed matter physicists. It is an alloy primarily made of Carbon and Iron and sometimes other elements which are used to tune its properties tailored to specific applications. Small amounts of exotic elements such as Yttrium ($\sim$ 0.1 %) are for instance added to enhance its high-temperature mechanical properties. Such engineering is crucial in development of next generation power reactors for instance. Versatility of steel makes it a strategic alloy. Beyond traditional alloying techniques rooted in materials optimization and engineering, modern physics has enabled engineering of materials like Steel beyond what was imaginable. Decarbonizing steel through composites, remain one of the most active areas fo research in Materials Engineering. In fact in the words of the International Energy Agency (IEA):

> *"Material efficiency contributes approximately 30% to the combined CO_2 emissions reduction."*

for steel, aluminum, and cement combined International Energy Agency (2023, 2019). Carbon Nanotubes (CNTs) are a class of quantum materials with extraordinary properties. Reinforcing Steel with such materials is an active area of research, crucial to

development of Fusion Micro-reactors or other applications, necessary for energy transition in the era of climate catastrophe. Figure 1 shows the potential for CNTs to fill in the micro-structural gaps in steel, making it less susceptible to radiation. Furthermore, such materials can reduce the carbon footprint in manufacturing Steel itself. In the following sections, first I will introduce Carbon Nanotubes, then I will move on to techniques in materials optimization and the design of CNT-reinforced Steel, followed by a discussion about the role of these exotic materials in decarbonization.

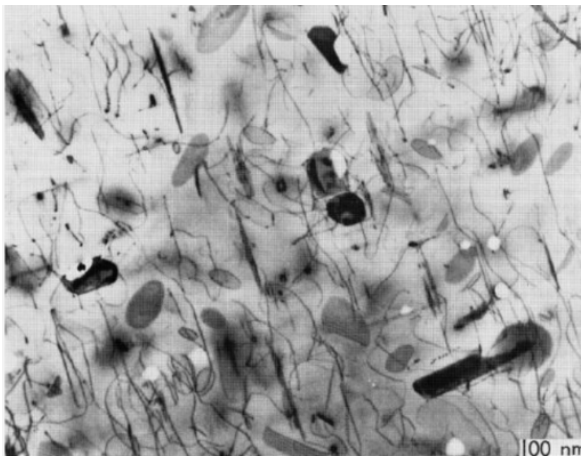

Figure 1. Visible micro-structures of Irradiated steel under Transmission Electron Microscope. CNTs have the potential to fill in those gaps, making steel less vulnerable to radiation.

2 PROPERTIES OF CARBON NANOTUBES (CNTS)

2.1 Introduction

Sheets of Graphene, when rolled into cylinders, exhibit extraordinary properties such as exceptional mechanical strength, high electrical conductivity, and unique thermal properties. These rolled sheets are called Carbon Nanotubes (CNTs). In 1985, Kroto et. al. Kroto et al. (1985) discovered a new form of carbon, called the C60 , which is a molecule made of carbon atoms and as a result, won the Nobel Prize in chemistry in 1997. It resembles the soccer-ball . In 1991 things took an interesting turn when Iijima discovered multi-walled CNTs (MWNT) Iijima (1991) and about two years later, made the observation of single-walled nanotubes (SWNT) Iijima and Ichihashi (1993). CNTs have similarities to graphene but behave rather differently. In fact, the way graphene is rolled (i.e. chirality) plays a significant role in the intrinsic properties of CNTs. This can be better seen in figure 2.

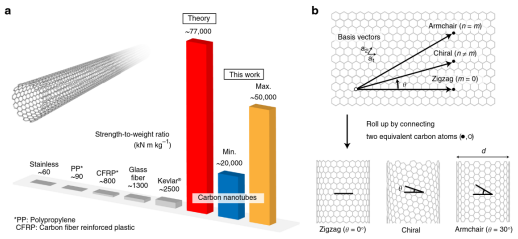

Figure 2. Chirality of CNTs. The way graphene is rolled plays a significant role in its properties Reich et al. (2008). Also, extraordinary mechanical properties of CNTs compared to other materials can be visualized. Adapted from Takakura et al. (2019a).

The Hamiltonian for a CNT is similiar to finding one for graphene, its parent material. In the tightbinding approximation, the Hamiltonian can be written as:

$$H = -t \sum_{\langle i,j \rangle, \sigma} \left(a^{\dagger}_{i,\sigma} b_{j,\sigma} + b^{\dagger}_{j,\sigma} a_{i,\sigma} \right), \tag{1}$$

where:

- t is the nearest-neighbor hopping energy,
- $a^{\dagger}_{i,\sigma}$ ($a_{i,\sigma}$) creates (annihilates) an electron with spin σ on sublattice A at site i,
- $b^{\dagger}_{j,\sigma}$ ($b_{j,\sigma}$) creates (annihilates) an electron with spin σ on sublattice B at site j,
- $\langle i, j \rangle$ denotes summation over nearest-neighbor pairs (visualized in figure 3).

Figure 3. The 3 nearest neighbor atoms in graphene to better visualize the hamiltonian.

2.1.1 Thermal and Mechanical Properties of CNTs.

Graphene has the highest intrinsic thermal conductivity but multilayer graphene is the most promising material for practical applications in thermal interface materials Balandin (2020).

Thermal conductivity of CNTs remains to this date, a controversial topic Bruns et al. (2021). Acoustic phonons are particularly responsible for lattice heat transport. While 2D graphene sheets and their derivative, CNTs show efficient heat transport properties Balandin (2011), external factors such as residual mechanical strain play a significant part in introducing errors to measurements. With propagation of these errors, the task of experimentally verifying the heat transport in such materials remain a challenge Bruns et al. (2021). It is noteworthy that the first experiments to study the thermal conductivity of graphene were performed at the University of California, Riverside Balandin et al. (2008).

Salvetat et al. (1999) : Mechanical Properties of Carbon Nanomaterials:

Thermal transport of CNTs is thought of as being a function of dimension, length and the temperature:

$$\kappa = \kappa(D, L, T) \tag{2}$$

The Fourier law is simply the gradient of the temperature and reads:

$$\mathbf{q} = -\kappa \nabla T \tag{3}$$

Where here, κ is a second order tensor.

The value of κ is also affected by the curvature and size of the carbon network Thomas et al. (2010). Size dependence plot of κ is shown in figure [4]. The temperature dependence of κ itself is shown in figure [5].

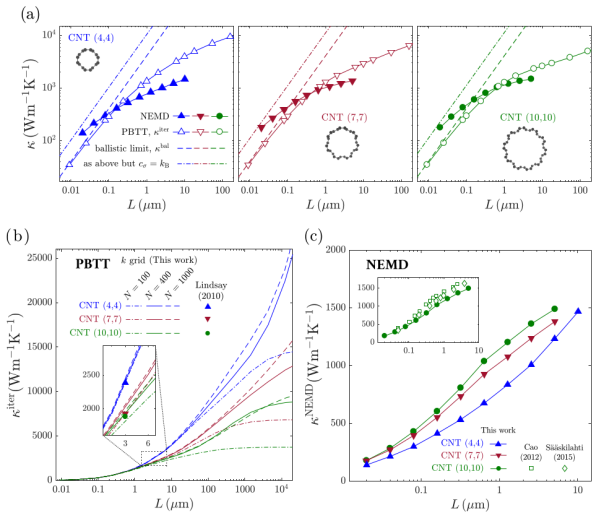

Figure 4. Size dependence of κ in CNTs at near room temperature, as predicted by simulations. (a) Increasing with CNT diameter - dashed: Quantum, dashed-dotted: Classical (b) Varying wave number grids with reference to data (c) Sim. results in log-linear scale with respect to data. Adapted Cao and Qu (2012).

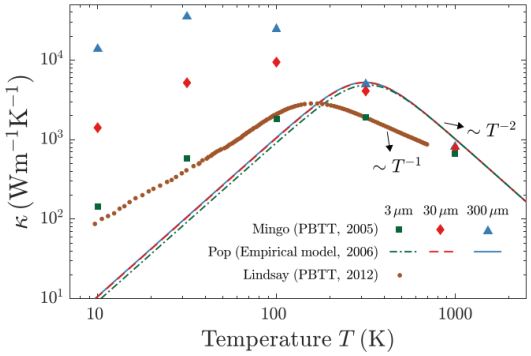

Figure 5. Temperature dependence of κ, Adapted from Ref. Mingo and Broido (2005); Lindsay and Broido (2012)

As additional long-wavelength phonon modes become accessible with the increase in length, the thermal conductivity of single walled CNTs are increased. This picture in effect suggests that contributions of electrons to the CNT thermal conductivity are generally considered to be negligible and the high thermal conductivities of CNTs can be simply explained by the long phonon mean free paths. However, there is a limit to this picture, and that length limit is about (100 *nm*), hereby called Λ for a diameter of 1 *nm*. So we take this length as a reference for our discussion:

$$\Lambda = 100\,nm$$

For tube-lengths longer than this, the phonon-phonon scattering rate increases which causes the phonons to practically diffuse before reaching the other end of the material. At this point, the thermal conductivity become length independent. It is noteworthy that with increasing diameter, this length also becomes shorter, as if the volume is constant [1]. When these CNTs are filled with water, an interesting phenomenon is observed. The length Λ becomes shorter. Although the exact analytical mechanism for this is unknown, their simulations furthermore show an overlap between vibrational degrees of freedom accessible to water Molecules and phonon modes (acoustic) in CNTs.

2.1.2 Mechanical Properties

Single-walled CNTs are predicted to have tensile strengths between 100 and 200 GPa (That of Steel is around 350 MPa), predicting the existence of a material around 1000 times stronger than steel. Yet, the strengths recorded in experiments are much lower and inconsistent. The strength depends on the chiral structure of the nanotube, with small-diameter, near-armchair nanotubes exhibiting the highest tensile strengths and is first reported in 2019 by Takakura et. al. Takakura et al. (2019b). See figure [2] for details.

2.1.3 Challenges In CNTs

CNTs exhibit extraordinary properties but the thermal conductivity of CNTs continues to be a subject of debate. Theoretical predictions of such properties through computational modelings are usually performed using techniques such as Molecular Dynamics (MD) and energy minimization computational techniques Han and Elliott (2007). Acoustic phonons play a key role in the movement of heat through the lattice of these materials. Although both 2D graphene and CNTs, demonstrate excellent heat conduction capabilities, external influences like residual mechanical strain significantly affect measurement accuracy. This strain introduces errors that propagate through the experimental data, making it difficult to confirm the heat transport characteristics of these materials..

Being able to predict materials properties through computational efforts such as machine learning Murphy (2022); Wei et al. (2019) might as well prove to be helpful in experimental efforts. In the remaining part, I briefly discuss some possibilities for future work. The degree to which the thermal conductivity of CNTs are sensitive to external perturbations is unknown. Contemporary and future research perhaps would shed light on this important aspect of research in determining the properties of these materials. Also, nuclear degree of freedom in Born-Oppenheimer (BO) approximation Born and Heisenberg (1985) is the last term in

$$E_T = E_{e.} + E_{vib.} + E_{rot.} + E_{nuc.} \tag{4}$$

Where the first term is electronic, second therm vibrational, and the third term rotational degrees of freedom. This suggests that in higher order phonon-phonon interactions, the nuclear degree of freedom becomes significant, resulting in possible deviations from the T^{-1} behavior. This in effect shows the degree of complexities in such calculations. Last, but not least, the role of electron-phonon interactions particularly becomes important in the case of non-equilibrium transport where phonons and electrons exchange momentum and energies. This is also not well understood to date. Finally, to put it in Balandin's words, "It is possible that the true "killer" application, or rather a range of applications, will come from graphene's phononic rather than electronic properties." Balandin (2020)

3 COMPUTATIONAL APPROACHES TO MATERIAL DESIGN

In modern days, material design is primarily conducted computationally. Although computationally expensive, new approaches have made such tasks more affordable. New advancements in Artificial Intelligence for instance, are pushing the limits of materials design to lengths previously not possible. The complexity of such tasks are usually reduced when physical laws are implemented in the design of models which can contribute to materials

[1] There are no references in the literature regarding this defined volume to be a constant and this picture is used for discussion purposes here. This behavior however is usually attributed to increase in acoustic phonon scattering in larger-diameter CNTs. See for instance: Thomas et. al. Thomas et al. (2010).

design. For instance, a physics equation by Rahemi-Hua Rahemi (2015) describes how the young's modulus of metals varies with the temperature. Implementing such laws into modeling and data assimilation, significantly reduce computational expenses, as the need for trial-error are diminished. Figure 7 shows a successful MCMC model performed on the Rahemi-Hua model, which determines the physical limits of tailoring a metal for high-energy applications.

3.1 Materials Optimization

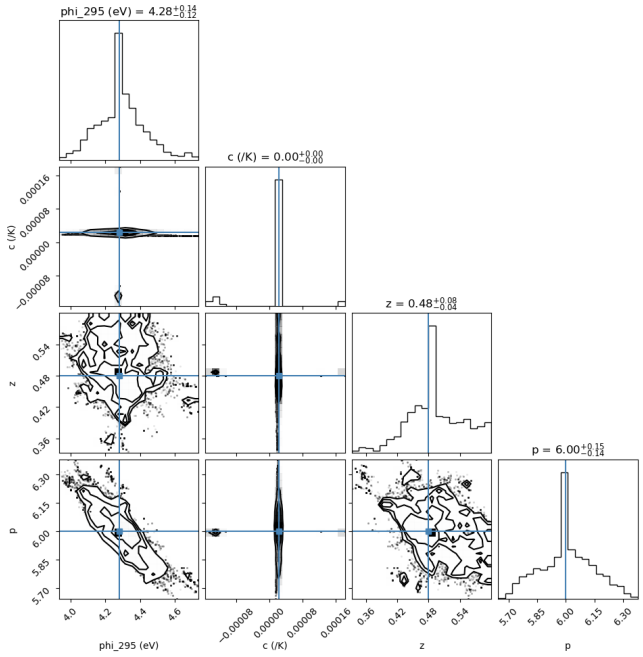

Figure 7. Markov Chain Monte Carlo simulation of the parameters in Rahemi-Hua equation of change in General Elastic Modulus $\Psi_T = -2\alpha\frac{K_B T}{\Psi_0}$, applied to elastic modulus of metals, demonstrating computational optimization of material properties. Rahemi (2020). The corner left plot in this figure shows how changing electronic parameters inside a metal (variable ϕ_{295} (Electronic work function of Aluminum at room Temperature) can tune the Elasticity parameter (varibale P).

3.1.1 Monte Carlo Markov Chain: Defining Log-Likelihood and Log-Prior

We want to know how well the model fits the data.

For Gaussian errors, the likelihood is:

$$p(y_j|\theta) = \prod_{j=1}^{N_j} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y_j - v(x_j,\theta))^2}{2\sigma^2}\right). \quad (5)$$

When taking the Log-Likelihhood, the product becomes a sum. Given $\sigma = 1$, it simplifies to

$$\log p(y_j|\theta) = A(-\frac{1}{2}\sum(y_j - v(x_j))^2) \quad (6)$$

Where A is a constant throughout the MCMC process.

3.1.2 Bayesian Context

In Bayesian Context, the Posterior distribution of the parameters given the data $p(\theta|y)$, which is our goal, is given as:

$$p(\theta|y) = \frac{p(y|\theta)p(\theta)}{p(y)} \quad (7)$$

$p(y|\theta)$ is the likelihood (How probable the observed data is under specific parameter values). $p(\theta)$ is our initial beliefs about the parameters. $p(y)$ is the Evidence, which is a normalizing constant, which can be ignored in MCMC since we are sampling ratios. So in order to find the posterior, we need to compute the likelihood, which determines how well a given set of parameters θ explains the data y.

3.1.3 Random Walk Metropolis Sampler

We have a uniform prior, where $p(\theta)$ is a constant if within bounds, and if not, zero. So log prior would be o if valid and $-\infty$ if not. The purpose of this is to constrain parameter ranges.

$$p(\theta|y) \propto p(y|\theta)p(\theta) \quad (8)$$

This algorithm implements the Metropolis-Hastings MCMC algorithm. Starting at an initial guess, we propose a new point $\theta' = \theta + S \cdot N(0,1)$ with S being the step scale. We then compute the log-posterior by taking the log of eq. 8, we arrive at:

$$\log p(\theta|y) \propto \log p(y|\theta) + \log p(\theta) \tag{9}$$

The outputs are chain of samples, log-posterior values and acceptance rate.

As of today, the topic of Brownian Motion is 120 years old (since Albert Einstein published his famous paper on this topic in 1905). The centennial anniversary paper on this topic was published in 2005, in [Hänggi and Marchesoni (2005). This topic in itself is so rich in literature that almost all aspects of Brownian motion are in fact studied. This however does not mean that this topic is completely "solved". For example, the role of quantum noise when several reservoirs of different nature (or temperature) are coupled to the system of interest. This might have potential applications in Atmospheric Sciences, where the role of temperature could play a role in determination of the final state of a perturbed system. Further examination of this phenomenon, however, is beyond the scope of this project and the scope of my research. In the remaining parts of this paper, I have addressed the problem proposed following through explanation of statistical aspects of this topic and how it relates to Gaussian processes.

3.1.4 Stochastic Sampling

In the realm of classical motions, stochastic models works satisfactorily. This can be realized through working out a stochastic process for a typical Brownian motion. Starting off with the Newtonian $\mathbf{F} = \dot{\mathbf{p}}$, where $\dot{\mathbf{p}}$ is the derivative of momentum. When m is a constant, one gets the famous $\mathbf{F} = m\mathbf{a}$. Making the model slightly more complicated by introducing a negating force in the other direction (for instance viscous force in the suspension of water molecules in the air for instance) we get

$$dv = -\alpha v dt + dW \tag{10}$$

Where α, the viscous friction coefficient is positive and W is the mathematical Brownian motion. We are interest in the position of the particle, x and $v = \dot{x}$, where $\dot{x}$ is the derivative of the position with respect to time. this motion is simulated by parametrization and setting

$$dt \approx \Delta t = 1 \tag{11}$$

$$dx \approx \Delta x = x_{k+1} - x_k \tag{12}$$

$$dv \approx \Delta v = v_{k+1} - v_k \tag{13}$$

$$dW \approx \Delta W \sim \mathcal{N}(0, \Delta I) \tag{14}$$

Rearranging, we arrive at:

$$v_{k+1} = v_k - \alpha v_k \Delta t + \Delta W_k \tag{15}$$

$$x_{k+1} = x_k + v_k \Delta t \tag{16}$$

This is an example of a simulation of a Brownian motion achieved with studying a stochastic process. Monte Carlo Sampling added to a Markov Chain built on a similar Brownian motion produces a MCMC model, as applied to Rahemi-Hua model and seen in figure for materials properties applications 7.

4 CNT-REINFORCED STEEL (NANO-COMPOSITE)

Carbon Nanotubes are many times stronger and at the same time, lighter than steel and other metals. Their assimilation into steel metal matrix is challenging but with if done properly, can enhance the properties of the resulting composite Radhamani et al. (2018).

CNT reinforced stainless steel composites when fabricated by laser powder bed fusion (LPBF) additive manufacturing, significantly improves the thermal conductivity of steel, making them suitable for high-temperature applications. Hassanzadeh-Aghdam et al. (2019).

However, the technical and economical constraints still make the production of such materials a challenging task. Re-inforcing polymore composites can create elastic modulus values in the range of 170-450 GPa, which could be boost up to 600 GPa with CNTs Esawi and Farag (2007).

5 LOWER CARBON EMISSION AND DISCUSSIONS

Steel production worldwide amount to more than 7 percent of anthropogenic emissions of carbon dioxide. Although Hydrogen-based direct reduced iron methods can replace CO_2 emissions in the Steel production chain significantly, green hydrogen production itself is energy-intensive and currently expensive. Green steel is also susceptible to newly introduced micro-defects not present in conventional steel. DPA (Displacement per atom) in these materials are usually different than those of conventional steel, making them not suitable for strategic applications. Electric Arc Furnace with scrap recycling method also faces scarcity of resources and over-reliance on electricity grids. CCUS technologies implemented in steel production lines are also problematic and costly, which could serve as transitional solutions for legacy plants only. CNT-reinforced Steel is therefore a more promising yet seemingly futuristic option when it comes to decarbonization. With enhanced material properties leading to material efficiency (e.g. tensile strength, corrosion resistance, weight reduction), the need for material needed for a given application can be reduced. Steel Corrosion is estimated to contribute to 5-10 percent of global CO_2 emission, due to the need to replace the corroded steel. Corrosion resistance is improved with the use of CNTs. These nano-tubes act as bridged between micro-cracks and enhance the steel-concrete bond in reinforced structures. CNTs still face several challenges, which need to be addressed before they can be commercialized. Further research and development is therefore required to overcome such challenges.

Advancements in Steel production is a global effort. Realizing the economical and strategic advantages this material produces, research and development sections of many countries focus on the evolution of steel. In terms of volume, the Asian market is currently the dominant player in the supply of steel. Implementing new technologies to improve materiel properties has the potential to offset carbon emission beyond the footprint in steel production itself (i.e. the 7 %). Lightweight transportation with robust and reliable materials can be made possible with implementation of advanced additive manufacturing such as production of CNT-reinforced steel. Although the production of CNTs themselves might produce carbon footprint, new production technologies can avoid or at least mitigate this issue Licht et al. (2019); Parmar et al. (2024).

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