FRACTURE PROPERTIES OF MULTIDIMENSIONAL CARBON-BASED MATERIALS

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Abstract
We perform steered molecular dynamics tensile studies [1] on carbon-based low dimensional materials including carbyne, cyclo[18]carbon, carbon nanotubes, and hybrid structures. We study the response of these materials to quantify the maximum stress, strain, and force required for fracture. We then use density functional theory to study the electron density distributions at different strains in low-dimensional materials to validate the molecular dynamics fracture predictions. This study predicts the fracture and mechanical properties of carbon-based low dimensional materials that will help with applications such as nanodevices and nanocomposites.

1. Introduction

Low dimensional carbon allotropes are a diverse group of materials that could have a significant impact on the future of nanodevices and nanocomposites. This group includes the one-dimensional chain of carbon atoms known as carbyne, which has been predicted to have a high specific strength and stiffness [2], a two-dimensional ring of carbon atoms called cyclo[18]carbon [3], and three-dimensional carbon nanotubes. This range in dimension of nanomaterials has various mechanical properties that affect their potential applications; carbyne is well suited for lightweight applications requiring high strength, and cyclo[18]carbon is suggested for use as an ultra-elastic O-ring [3]. Combinations of the materials, such as the use of carbon nanotubes to encapsulate carbyne and a cyclo[18]carbon and carbyne hybrid, could also present different mechanical properties. These mechanical properties will also affect how these low dimensional materials fracture, which is necessary to determine prior to application in nanodevices. This study predicts the mechanical and fracture properties of low dimensional carbon-based materials.

2. Results

We investigate the mechanical and fracture properties of carbyne, cyclo[18]carbon, carbon nanotubes with and without encapsulated carbyne, and hybrids of carbyne and cyclo[18]carbon in which we use one, two, and three rings of cyclo[18]carbon. During steered molecular dynamics tensile tests, we determine that carbyne requires the most force to fracture, though the fracturing strains for the chain, carbon nanotubes, and encapsulated carbyne are quantitatively similar. The cyclo[18]carbon requires the least force to fracture, though it withstands the maximum strain of approximately 50% before the first C-C bond break occurs. We also find that carbyne fractures at a higher stress than their hybrid counterparts, and carbyne encapsulated in a carbon nanotube will have approximately the same fracture properties as the carbon nanotube without carbyne.

During the tensile tests, the hybrid structures undergo bonding and structural transformations when they surpass an initial transforming strain. The cyclo[18]carbon closest to the atom being pulled during the steered molecular dynamics begins to unravel from a two-dimensional ring to a one-dimensional chain after the first bond transformation occurs. This process is indicated by the multiple peaks in the force and strain relationship of the hybrid structure with one ring that is shown in Fig. 1. Interestingly, only the hybrid with one ring is able to fully transform into a chain of carbyne with the same high fracture force of carbyne before the sample is fractured. The hybrids with two and three rings fracture before becoming a one-dimensional chain.

We use density functional theory to investigate the electron density of the hybrid cyclo[18]carbon and carbyne structures at and prior to their transforming strains to validate the fracture processes observed during the molecular dynamics study. Using self-consistent field calculations, we create electron density plots for the hybrid structures and focus on the bonds in the right-most ring of the materials, as this is where the beginning of the ring unravelling process occurs at the strain of transformation. We find that the atoms connecting the ring and chain have a low electron density compared to other atoms in the hybrid structure. The change in bond lengths in steered molecular dynamics results are related to the electron density distribution results in DFT, thus validating the fracture process.

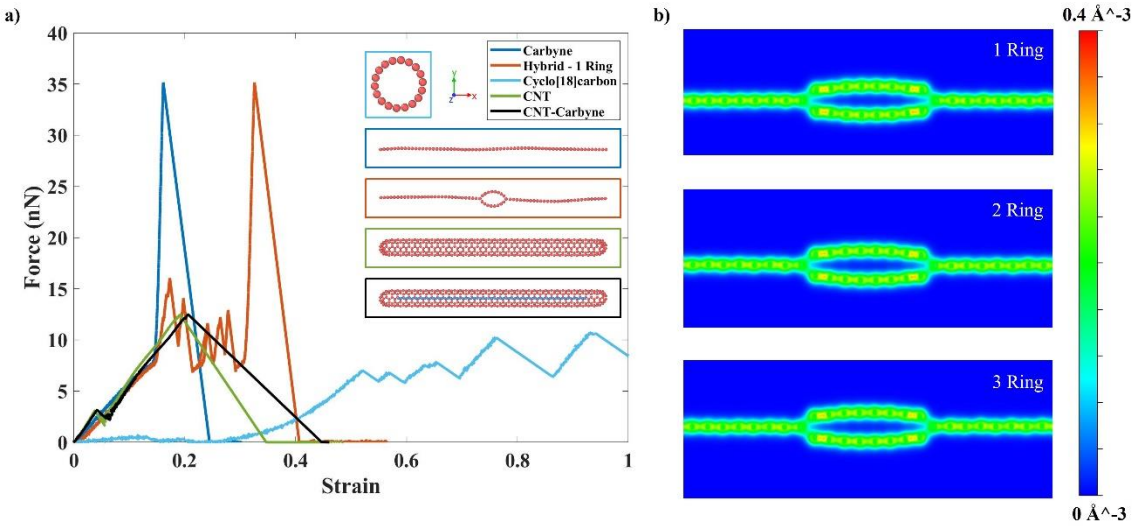

Fig. 1 – a) Force and strain relationship for carbyne, cyclo[18]carbon, a carbon nanotube (CNT), carbyne encapsulated in a CNT, and a cyclo[18]carbon and carbyne hybrid with one ring, b) Electron density of the right-most ring of the hybrid cases with their transforming strain

3. Conclusions

Using a combination of steered molecular dynamics and density functional theory methods, we investigated the fracture of a range of carbon-based multidimensional materials in response to tensile strain. We find that carbyne requires the most force to fracture at a strain similar to those of the other structures excluding cyclo[18]carbon, which has the highest critical strain and lowest maximum fracture force, and the hybrid structures. Hybrid cyclo[18]carbon and carbyne structures do not improve the strength or elasticity of otherwise isolated carbyne and cyclo[18]carbon, respectively. However, the hybrid with a single ring presents an interesting property of transforming into carbyne and delaying fracture.

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References

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