Transfer-to-Excellence (TTE) Program

Modeling and Calculating Graphene Straintronics

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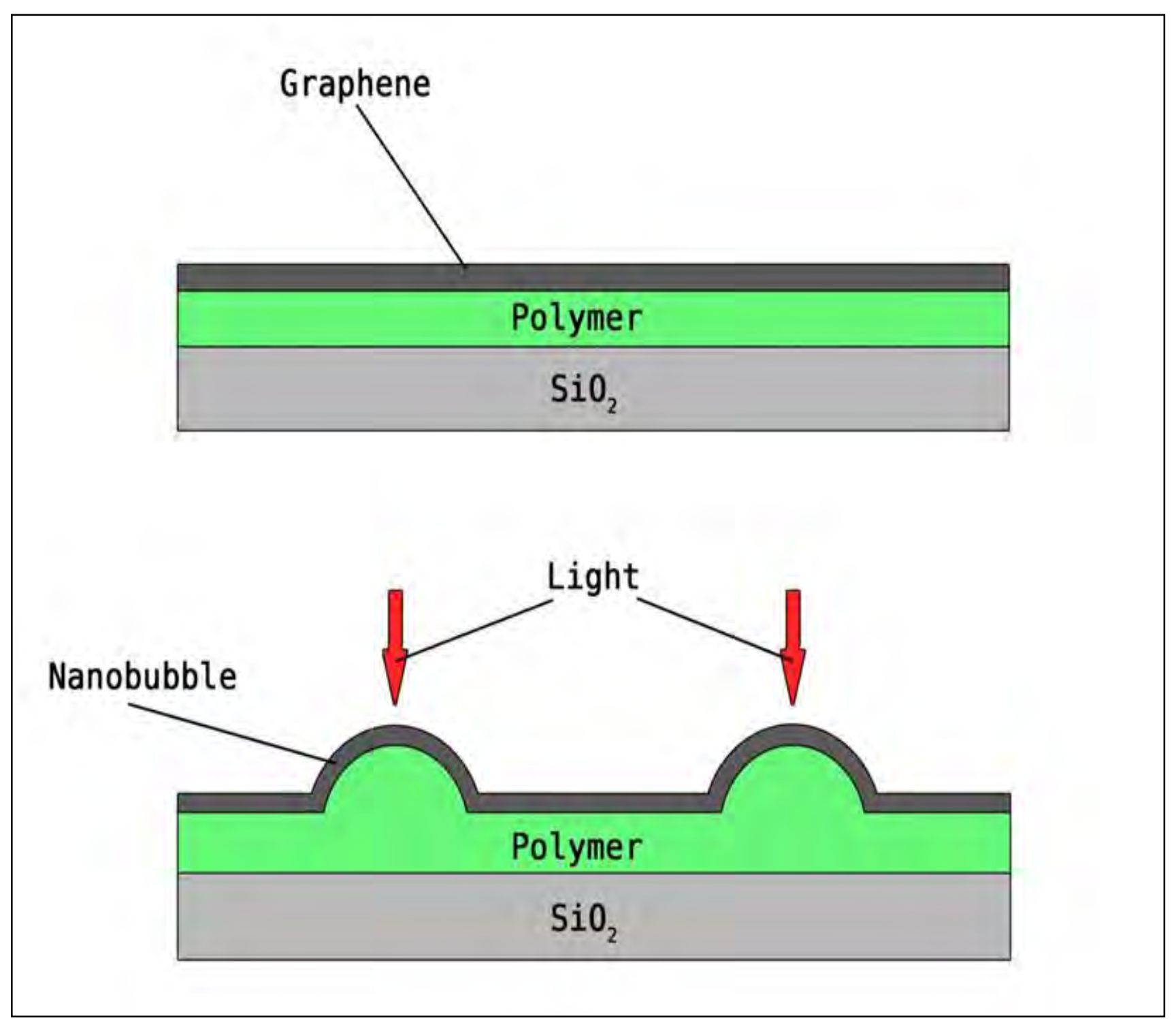
Abstract

The process of straining graphene in particular ways has been shown to produce graphene nanobubbles exhibiting strong pseudo-magnetic fields. A new technique involving light reactive polymers may provide greater control over nanobubble production. This new technique requires graphene to be accurately strained to a specific percentage by the deformable polymer underneath. Calculation and detailed modeling of the polymer's expansion, and the resulting strain on the graphene, can clue us in to the ideal conditions for the creation of nanobubbles in graphene. Finite element analysis of the elastic strain on the graphene sheet at and around the nanobubbles will allow us to create the previously established ideal strain parameters and control nanobubble production with great accuracy.

Introduction

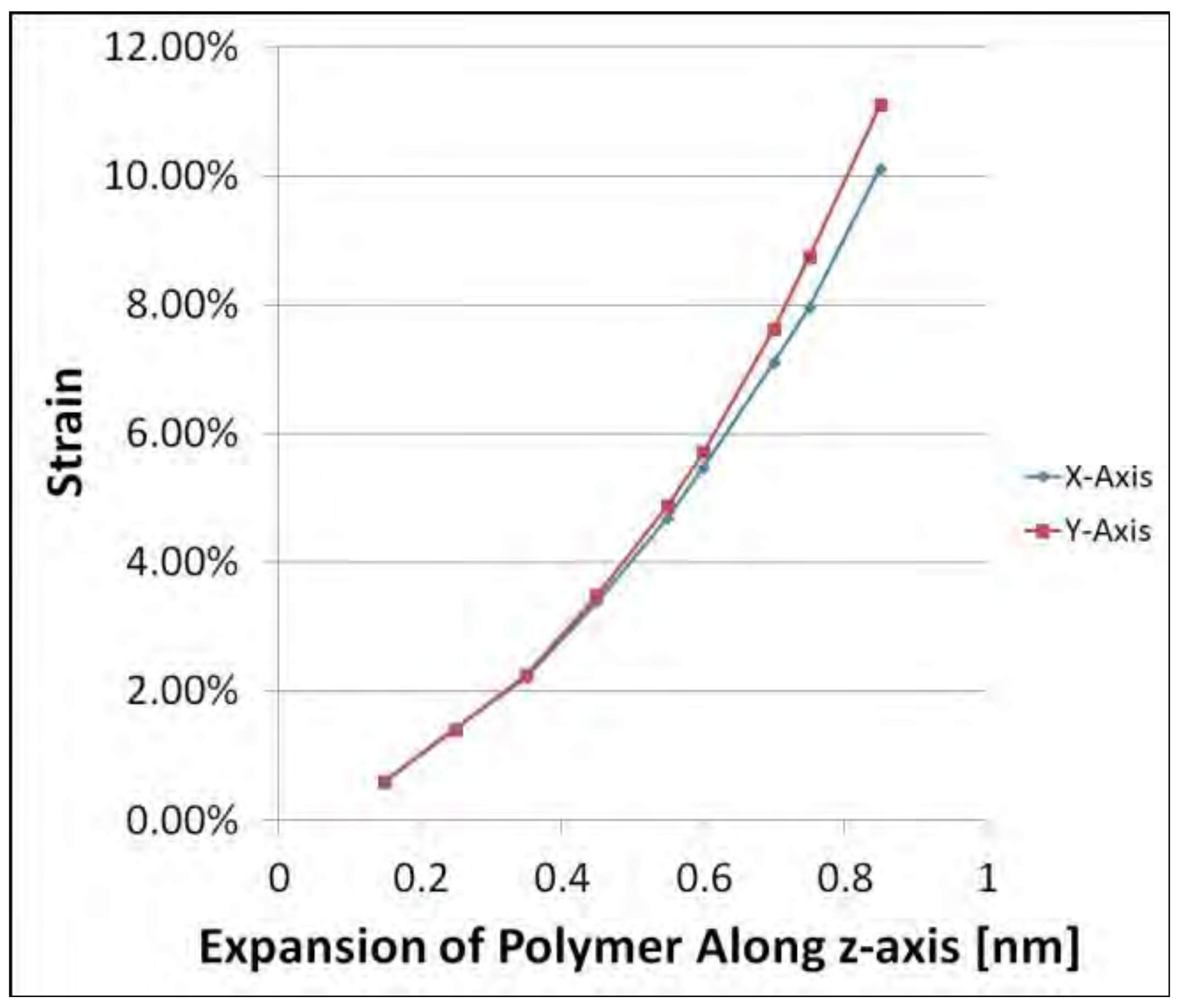
Motivation

- Layers of graphene one carbon atom thick have far reaching implications in the world of computing and electronics and have researchers all over the world working to harness its potential as a powerful semi-conductor. Straintronics, or strain engineering, has been shown to create pseudo-magnetic fields in graphene and is one promising method for controlling the flow of electrons.
- The capability to engineer precise strain percentages and geometries into graphene with the use of controlled nano-bubble deformation will no doubt move us closer to powerful graphene-based electronics.



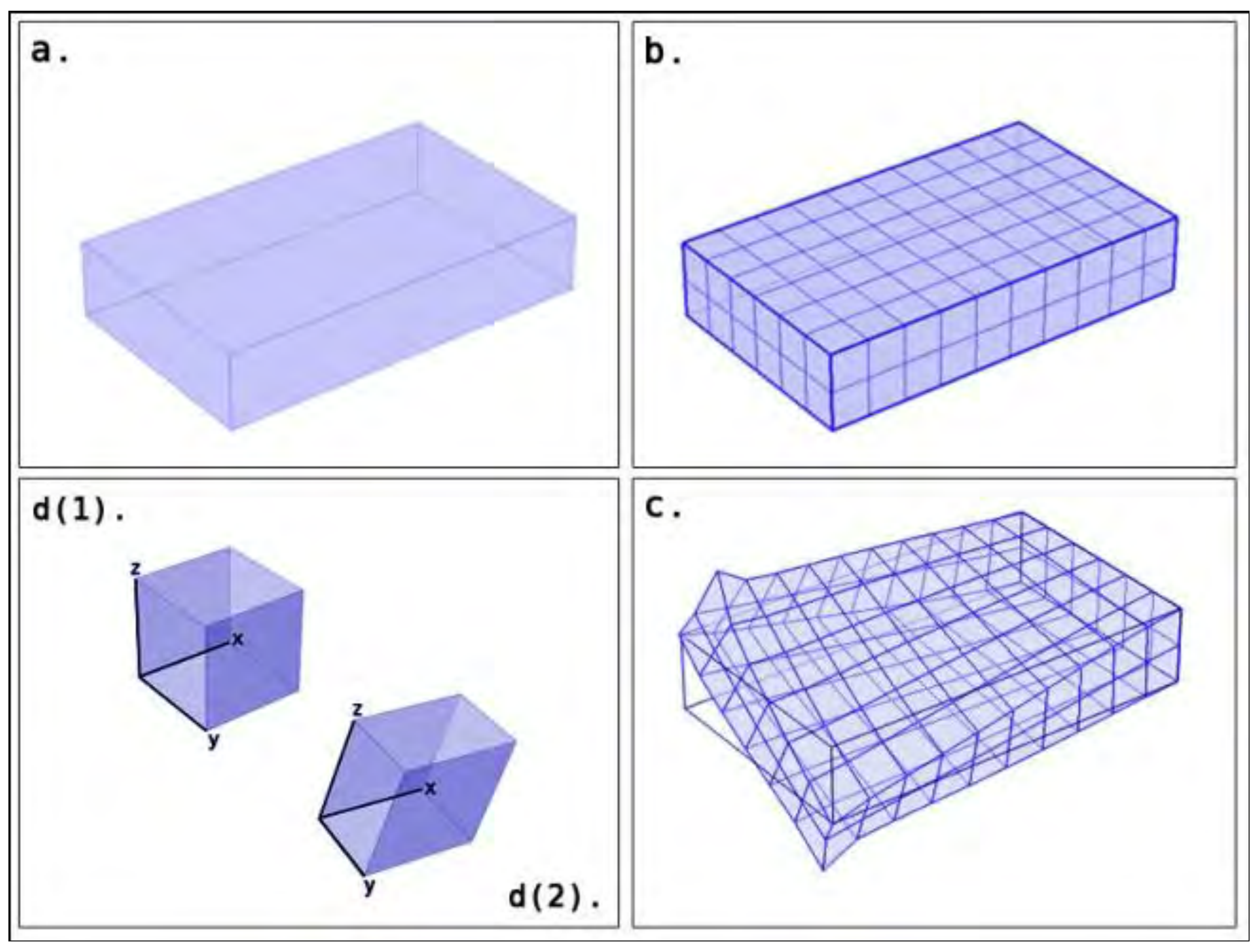
Strain of graphene by light reactive PMMA-based deformable polymer.

Strain Vs. Vertical Polymer Expansion



Methods

Finite Element Analysis is the process of modeling structural behavior by breaking a structure down into smaller elements for individual analysis. The elastic characteristics of graphene have been compiled and finite element analysis has been used to model and analyze the deformation and resulting strain of a sheet of graphene.



A solid block before (a) and after (b) it is broken down into elements. (c) A solid block after being deformed with elements and nodal points displaced. An individual element before (d1) and after (d2) being deformed.

References

F. Guinea, M. I. Katsnelson, and A. K. Geim, "Energy gaps and a zero-field quantum Hall effect in graphene by strain engineering," *Nature Physics*, vol. 6, no. 1, pp. 30-33, Sep. 2009.

Support Information
This work was funded by
National Science Foundation
Award ECCS-1157089

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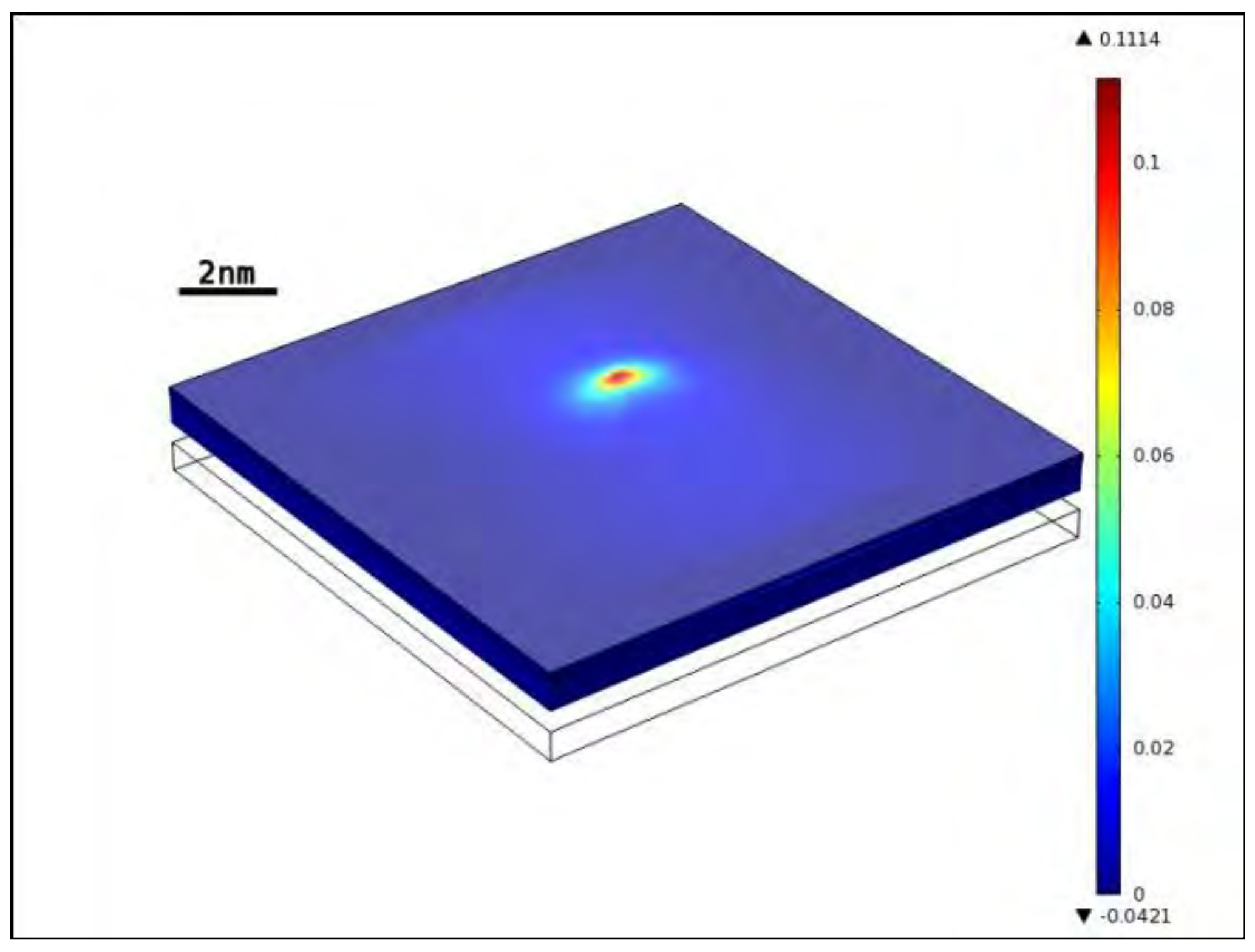
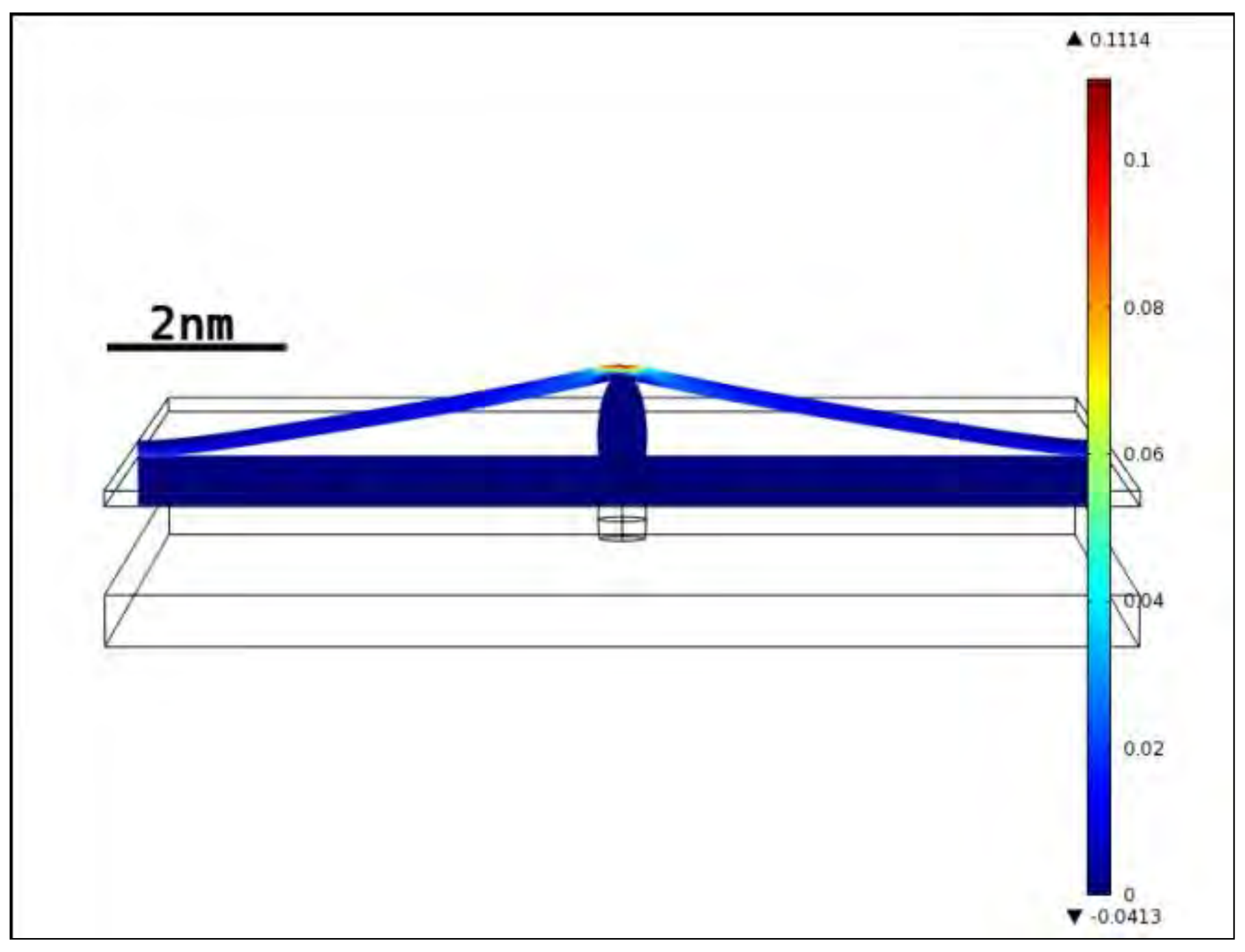
Strain Model at 0.85 [nm] Polymer Expansion



3-D model of graphene with max strain percentage of 11.1% from controlled deformation of light reactive polymer.



Cross-sectional slice of graphene with 0.85 nm of vertical polymer expansion.

Conclusion and Future Directions

Previous experiments have established an ideal pseudo-magnetic field in graphene at a strain of 10%. Based on experimental modeling, this ideal strain could be achieved with as little as 0.8-0.9 nm of vertical polymer expansion.

Future research should look into different strain geometries and the effects of multiple strain points. Three-point strain should produce the trigonal strain geometry necessary to create constant pseudo-magnetic fields in graphene as shown in previous research.

Acknowledgements

Kacey Meaker, Mike Crommie, COINS, and the TTE REU program