Negative Poisson's Ratio in Defected Schwarzites

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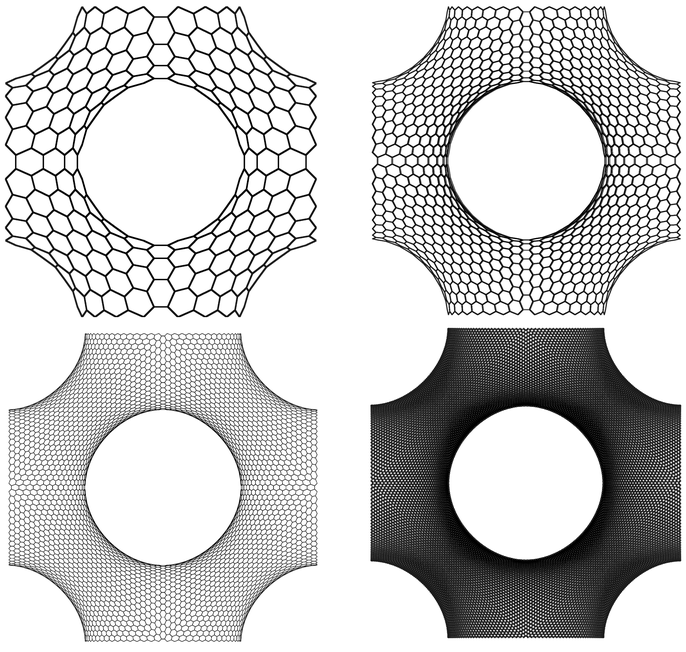
Introduction

Schwarzites are a family of analogs of porous graphene and have shown a rich variety of mechanical and electrical properties. One property of interest is Poisson's ratio, the ratio of transverse strain to axial strain. We calculated Poisson's ratio for Schwarzites with Primitive surfaces, which have Poisson's ratios of about 0.3-0.4. However, we can tune the Poisson's ratio by introducing Stone-Wales (SW) defects. We have shown that negative Poisson's ratio can be achieved in some stable defected Schwarzites, opening the possibility to synthesize auxetics, material with high energy absorption and high resistance to fracture, in the near future.

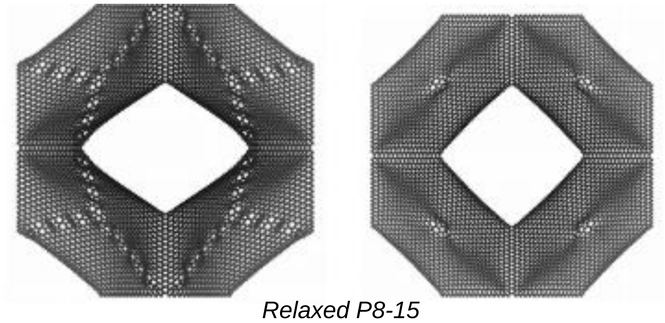


Schwarzites with Primitive Surfaces
Top Left: P8-3, Top Right: P8-7, Bottom Left: P8-15, Bottom Right: P8-31

A Stone-Wales defect is a crystallographic defect involving the rotation of a carbon bond by 90 degrees, resulting in the transformation of 4 hexagons into 2 heptagons and 2 pentagons. In our case, one stated defect is a triple SW defect (3 defects around a central hexagon). We placed triple SW defects on each corner of the cubic cells symmetrically, totaling to 8 SW defects for each represented triple SW defect.

Methods

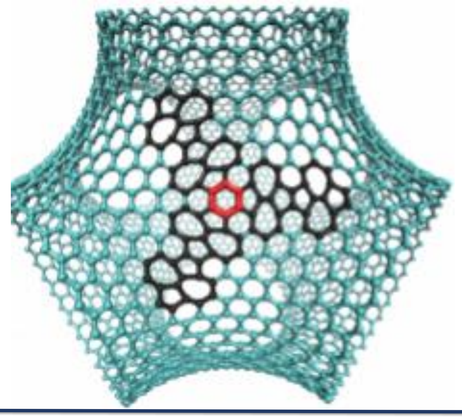
We used the primitive surface family of Schwarzites as it favors a smaller Poisson's ratio and is much more energetically and elastically stable. Triple SW defects were added to four different Primitive surface structures with varying sizes: P8-3 (768 atoms), P8-7 (3072), P8-15 (12,288), and P8-31 (49,152).



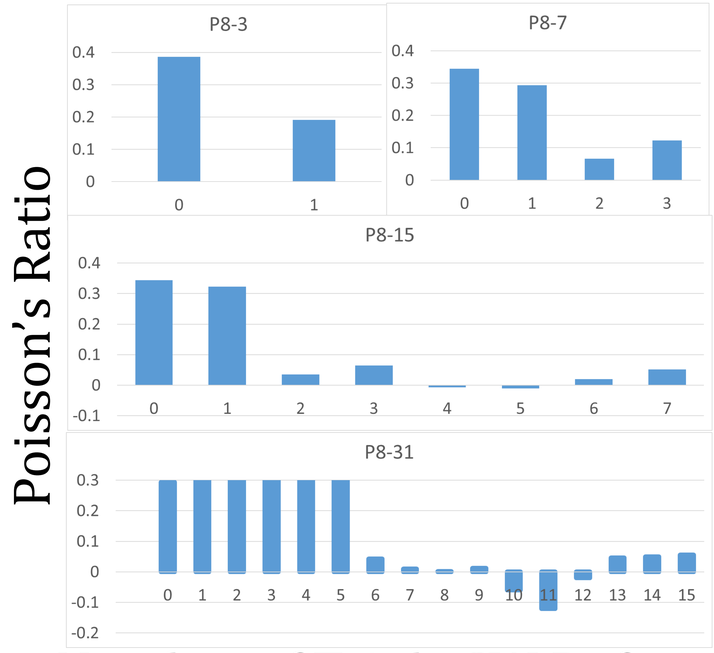
Relaxed P8-15
Left: P8-15 with 7 defects, Right: P8-15 with 2 defects

Using software package, LAMMPS (Large Atomic/Molecular Massively Parallel Simulator) , we ran molecular dynamics simulations on the cubic cells of the four structures. The structure is initially relaxed by undergoing energy minimizations. This is a process of finding an arrangement of space for a collection of atoms where the net-atomic force on each atom is close to zero. Perturbations are then applied and deformations performed to obtain the elastic constant tensor. From the elastic constants, we calculated Poisson's ratio. For our calculations, the REBO potential was used.

2 Triple SW Defects



Results and Discussion



With the introduction of SW defects, Poisson's ratio decreases; both P8-15 and P8-31 have structures with negative Poisson's ratio. The lower Poisson's ratio is due to the lower lattice parameter resulted from the defects. In the case of P8-15 and P8-31, a number of defects must be added before there is a significant decrease in Poisson's ratio. However, if too many are added, the increase of local curvature will cause Poisson's ratio to increase instead. All of the calculated structures meet the Born Stability Criteria for cubic cells giving the possibility of synthesized carbon auxetic material. Other surface families of Schwarzites such as Diamond, Gyroid, or IWP should also be studied to further understand the role of SW defects in a Schwarzite's Poisson's ratio.

References:
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2. H. Terrones, A. Mackay, The geometry of hypothetical curved Graphite structures, Carbon 30 (8) (1992) 1251-1260.
3. S. Plimpton, Fast Parallel Algorithms for Short-Range Molecular Dynamics, J Comp Phys, 117, 1-19 (1995).

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