Poisson's Ratio of defected Schwarzites

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Abstract

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 syntesize auxtics, material with high energy absorbtion and high resistance to fracture, in the near future.

I. Introduction

Poisson's ratio is the ratio of transverse strain to axial strain. If a material with high Poisson's ratio, such as rubber with a value of 0.5, is strained in the z and y-axis, the material will expand and thicken in the x-axis. Whereas cork, which has a near-zero Poisson's ratio, will barely expand when under the same strain. This makes cork the perfect material for wine bottles which have to withstand the pressure from within the bottle. There are also material with negative Poisson's ratio, known as auxetic material. When auxetics are put under the same strain in the z and y-axis, the material contacts, instead of expanding. Likewise, when the material expands in the z and y-axis, the material thickens in the x-axis. This property allows auxetics to have high energy absorption and high resistance to fracture making it a very useful material. It is believed that many materials with negative Poisson's ratio are unknown and most material are either anisotropic or foam. Negative Poisson's ratio can be found in defected Schwarzites, and if we find that they are also stable, there is also a possibility of synthesizing them.

Schwarzites are a family of graphene (a sheet of carbon) with negative Gaussian curvature. The negative Gaussian curvature results in unique mechanical and electronically properties, including Poisson's ratio. Schwarzites with triply periodic minimal surfaces (TPMS), which include Primitive surfaces, have had their properties calculated [2]. This paper focuses mainly on Primitive surfaces as they favor smaller values of Poisson's ratios and are more energetically and elastically stable.

It has been shown that there is a negative correlation between the size of the carbon cubic cell and its Poisson's ratio [2]. We have taken the correlation further to see if this remains true for even larger structures, specifically structures with Primitive surfaces. While the Carbon paper calculates mechanical properties up to P8-7 which has 3072 atoms, we will calculate the Poisson's ratio of P8-15 (12,288 atoms) and P8-31 (49,152 atoms). We have a simple naming convention for the various Schwarzites. First, the abbreviated letter 'P' which stands for Primitive (we will not be dealing with the other TMPS families), next an '8' to indicate the presence of octagonal rings. The cell itself only contains hexagons (as well as pentagons and heptagons if defects are added), but between two cubic cells is a band of octagons and hexagons (see Figure 3). The '8' is then followed by the minimum number of hexagons to separate two octagons. Notice, as the last number increases, the more atoms the structure contains. P8-1 only contains 192 atoms while P8-31 has 14,192 atoms.

The structure size only has a slight effect on the Poisson's ratio (less than half a percent difference between P8-7 and P8-15). However, we can tune the Poisson's ratio significantly by adding Stone-Wales defects (SW defects). SW defects have been to shown to alter the mechanical and electrical properties of various carbon structures [1]. A SW defect is put into place by rotating a carbon bond 90 degrees resulting in turning four hexagons into two pentagons and two heptagons (See figure). A structure with a defect is denoted by 'D3'. The '3' indicates the addition of 3 SW defects. We surround a hexagon with the defects leaving a gap in between (SEE FIGURE). To add another triple defect to a structure we attach another defect to the pentagon end of the previous defect (SEE FIGURE). Also, defects are applied to each corner of the cubic cell, so '1 defect' is actually 24. For instance, P8-15 D3-3 has 3 triple SW defects at each corner, making a

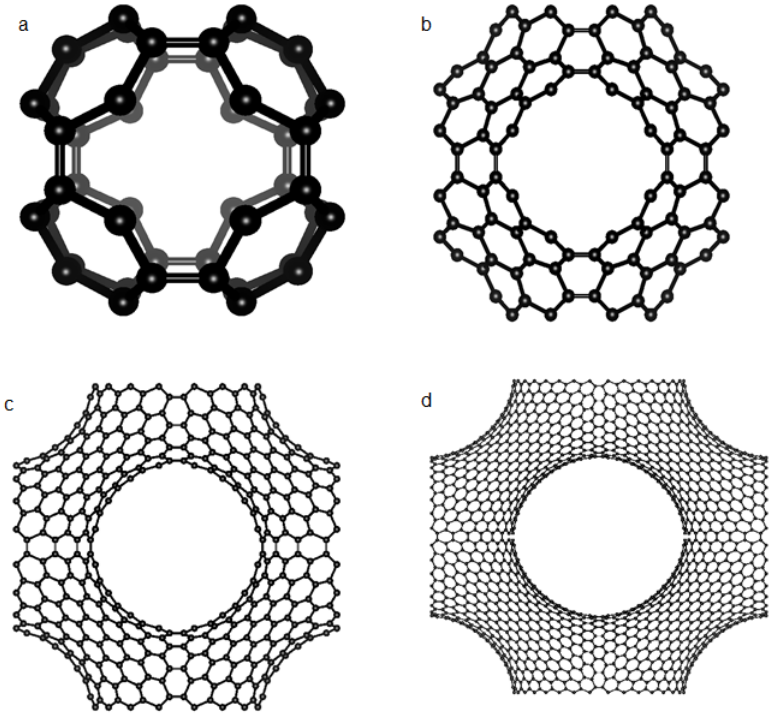


Figure 1: Schwarzites with Primitive Surfaces. a) P8-0. b) P8-1. c) P8-3. d) P8-7.

total of 72 defects.
(see Figure 1).

$$C_{11} - C_{12} > 0; C_{11} + 2C_{12} > 0; C_{44} > 0 \quad (1)$$

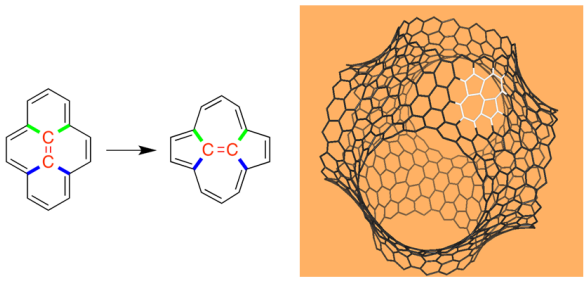


Figure 2: Bonds around two carbon atoms are rotated 90 degrees (left). Stone-Wales defect on P8-3 (right).

The goal of the paper is to find a Schwarzite that exhibits negative Poisson ratio and is stable. We can only synthesize a Schwarzite into auxetic material if it is stable. To meet the conditions of stability, the Schwarzite must pass the Born Stability Criteria (BSC). For a cubic crystal, such as a Schwarzite, the BSC is well-known (see Equation 1)[3]. C_{ij} comes from the Elastic Constant Tensor which also used to solve for the Poisson ratio. In this paper, we compute C_{11}, C_{12}, C_{44}, and the Poisson Ratio for Primitive Surfaces with or without Stone-Wales defects.

II. Methods

There are various types of Primitive structures and we will introduce the naming convention.

All calculations are done via the Large Atomic/Molecular Massively Parallel Simulator (LAMMPS). We chose to use this code because of its capability to handle larger atom structures. With the introduction of P8-31 which has 49,152 atoms, we needed a fast parallel engine for molecular dyanamics. LAMMPS allows the customization of which calculations to use and disregards any others which has little to no significance to our interests. For our purposes, we use LAMMPS to first relax the carbon cubic cell, undergoing an energy minimization. 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. To do this, we use the Reactive Bond Order (REBO) to find the potential energy of covalent bonds and intermolecular forces. As seen from Figure 4 below, a relaxed structure is flatter as it becomes more graphene-like. With the introduction of defects, however, the structure produces ripples around the area where the defects are.

After the structure has been relaxed, the code applies

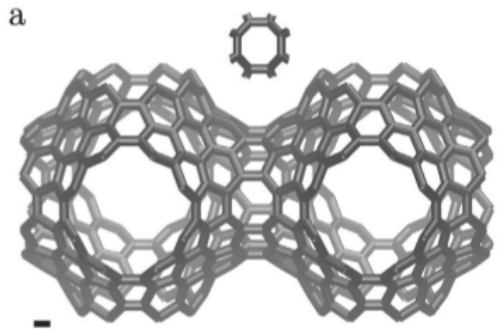


Figure 3: Two P8-1 Cubic Cells connected by an octagonal ring. Each octagon in the ring is separated by 1 hexagon.

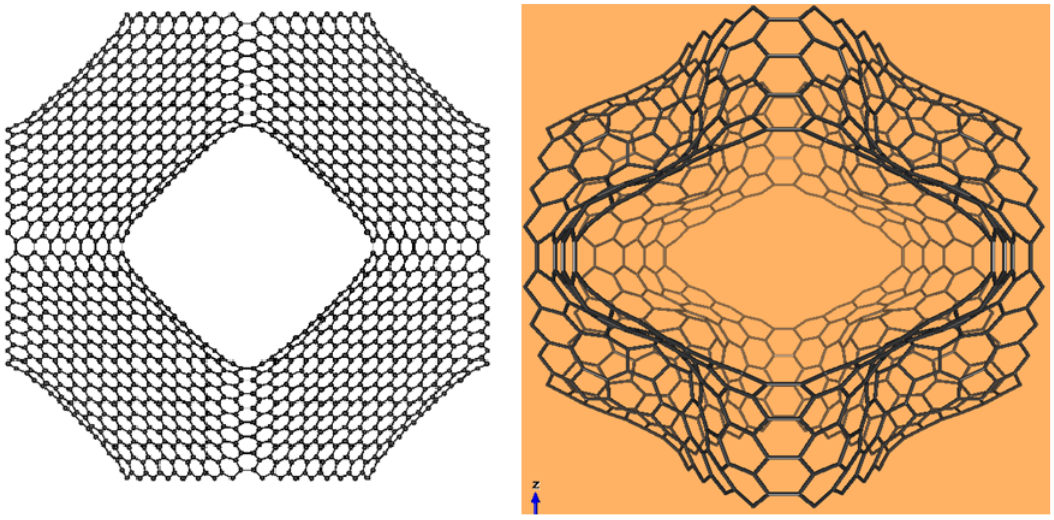


Figure 4: Relaxed P8-7 without defects (left). Relaxed P8-3 with 3 defects

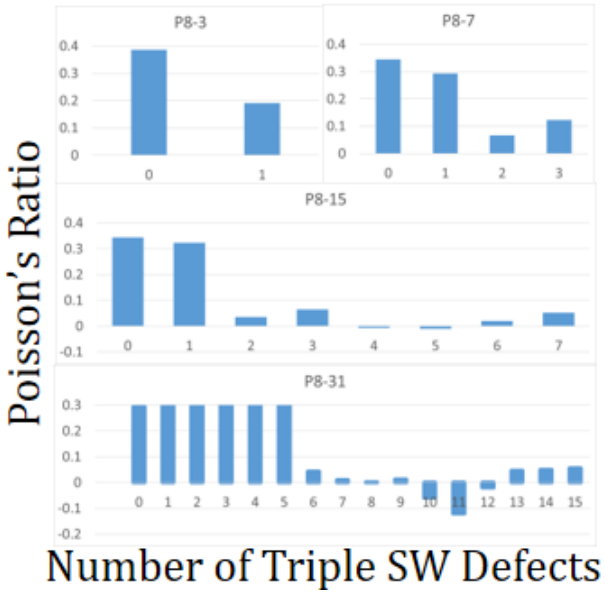
perturbations on the structure to calculate Elastic Constant tensor, which is then used to check the Born Stability Criteria and the Poisson ratio.

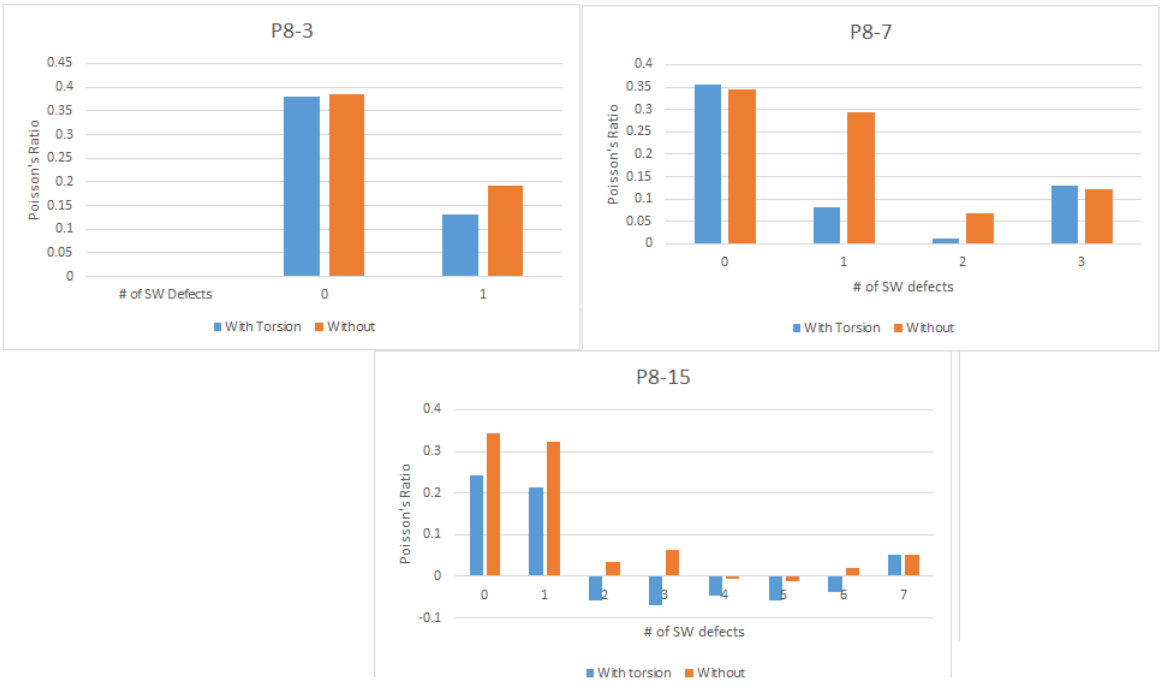
III. Results and Calculations

(see Figure 5). We believe the ripples caused by the defects are the largest factor in changing the structure's mechanical properties and this is because the ripples cause a decrease in the structure's lattice parameters. Table 1 shows the C11, C12, and C44 components of the Elastic and verifies that all of these structures meet the Born Stability Criteria. The table also shows the Poisson ratio of each structure. As the structure becomes larger (more atoms), Poisson's ratio decreases. Also, with the increase of the number Stone-Wales defects present, Poisson's ratio lowers.Both P8-7 D3-1 and D3-2 have near zero Poisson's Ratio. Moreover, P8-15 D3-2 and D3-3 have negative Poisson's ratio.

III.I. Torsion Potential

The calculations were done using the REBO potential, but some calculations were done with the addition of Torsion Potential. With the addition of the Torsion potential, the ripples of the defects are much more defined. This resulted in lower Poisson's ratio in most structures (See Figure). In P8-15, without the Torsion potential, only the structures with 4-5 defects are negative, but with it, structure with 2-6 defects are negative. Although Poisson's ratio were on average smaller, the trend is still the same. As the number of defects increase, the Poisson's ratio becomes smaller, but after a certain number of defects the Poisson's ratio begins to increase. Interestingly, when the Poisson's ratio begins to rise, the structure that underwent the Torsion potential has a larger Poisson's ratio (with the exception of P8-15 D3-7 which has the exact same Poisson's ratio as its counterpart). We believe this is because using only the REBO potential does not fully relax the structure. It is also interesting to note that the addition of the Leonard-Jones Potential may also have an effect on the structures and their Poisson's ratio.





III.II. Note about P8-31

Strutures with more than 6 defects the P8-31 series were not fully relaxed. Normally, for a cubic cell, the elastic constant tensor follows several rules: $C_{11} = C_{22} = C_{33}$; $C_{12} = C_{13} = C_{21} = C_{31}$; $C_{44} = C_{55} = C_{66}$. For fully relaxed structures, there would only be a difference in the 6th decimal place for equal constants; however, for P8-31 D6 and up, there is a difference in the 2nd decimal place.The easiest solution would be to let LAMMPS program run more force evaluations, but doing so causes a longer run time.

IV. Conclusion and Next Steps

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 critical 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

Table 1: Table for all cubic cases of Schwarzites with and without defects examined in this paper. The elastic constants (C_{11}, C_{12}, C_{44}) is given as well as Poisson's ration (ν)

	C_{11}	C_{12}	C_{44}	ν
P8-0	268.92	185.64	58.98	0.408
P8-1	147.29	99.37	79.66	0.403
P8-3	54.74	34.39	43.14	0.386
P8-3 D3-1	28.65	6.94	36.12	0.195
P8-7	22.46	11.82	20.47	0.345
P8-7 D3-1	17.14	7.11	21.28	0.293
P8-7 D3-2	9.54	0.68	15.00	0.067
P8-7 D3-3	9.45	1.32	13.89	0.122
P8-15	6.11	1.95	8.31	0.24
P8-15 D3-1	8.18	3.89	8.95	0.322
P8-15 D3-2	4.06	0.15	7.32	0.036
P8-15 D3-3	4.40	0.30	7.86	0.064
P8-15 D3-4	3.61	-0.03	5.92	-0.007
P8-15 D3-5	3.84	-0.04	7.00	-0.011
P8-15 D3-6	3.82	0.08	6.58	0.020
P8-15 D3-7	3.76	0.20	5.60	0.052
P8-31	2.02	0.83	3.32	0.293
P8-31 D3-1	3.08	1.32	3.49	0.300
P8-31 D3-2	2.56	1.17	3.45	0.308
P8-31 D3-3	2.67	1.19	3.49	0.309
P8-31 D3-4	3.28	1.50	3.54	0.314
P8-31 D3-5	5.17	2.78	5.73	0.326
P8-31 D3-6	1.43	0.07	3.03	0.043
P8-31 D3-7	0.94	-0.19	2.83	-0.046
P8-31 D3-8	0.73	-0.24	2.69	-0.060
P8-31 D3-9	0.69	-0.29	2.68	-0.074
P8-31 D3-10	0.66	-0.31	1.78	-0.101
P8-31 D3-11	2.47	1.33	3.67	0.053
P8-31 D3-12	3.60	1.54	3.33	0.123
P8-31 D3-13	4.89	1.98	3.66	0.242
P8-31 D3-14	5.33	2.41	5.58	0.309
P8-31 D3-15	3.74	1.90	4.37	0.337

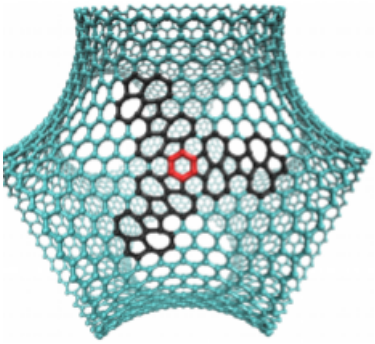


Figure 5: A double triple Stone-Wales defect (D3-2). Three Stone-Wales defects are connected by a hexagon in the center. This figure has '2' triple Stone-Wales defects since each protrusion has 2 Stone-Wales defects.

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.

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References

[1] N. Chandra, S.Namilae, and C. Shet. Local elastic properties of carbon nanotubes in the presence of stone-wales defects. *American Physical Society*, 69 (9), 2004. doi: 10.1103/PhysRevB.69.094101.

[2] David C. Miller, Mauricio Terrones, and Humberto Terrones. Carbon. *Elsevier*, 435(96):1191–1199, 2016. doi: 10.1016/j.carbon.2015.10.040.

[3] F. Mouhat and F.X. Coudert. Necessary and sufficient elastic stability conditions in various crystal lattices. *Phys.Rev.B90*, (22), 2014. doi: 10.1103/physrev.90224104.