

EVALUATING THE ELASTIC PROPERTIES OF POROUS SILICON AND POROUS SILICON SUBJECTED TO POLYMER TREATMENT

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ABSTRACT

The performance of materials in many engineering applications is significantly influenced by their mechanical behavior. Due to its special nanoscale structure and potential for a variety of uses, including microelectronics and sensors, porous silicon has become a material of interest. To realize its full potential, it is essential to comprehend and improve its mechanical qualities. Polymer treatment is a viable method for enhancing porous silicon's mechanical properties. Because of their mechanical adaptability and plasticity, polymers are a good choice for altering the characteristics of porous silicon. We seek to examine the effects of various treatments on the elastic properties of porous silicon, such as stiffness and resilience. In this study, we conduct a thorough analysis of the elastic characteristics of porous silicon that has not been treated and porous silicon that has been modified using polymers. With chances for innovation and technological advancement, our study aims to offer useful insights into the possible enhancements and applications of these materials in the fields of materials science and engineering.

The chapter describes the theoretical calculation of elastic properties of porous silicon and polymers treated porous silicon. The Elastic properties of porous silicon and polymers treated porous silicon were also depending upon the porosity. It is concluded that the theoretical calculation is a simple way to confirm the experimental results.

Keywords: Porous Silicon (PS), Polymers treated porous silicon, Elastic Property, Etching time, PMMA & PVC Concentrations

1. INTRODUCTION

To understand the porosity and the energy gap dependence of the elastic properties of PS, will first say general features observed in theories for the elasticity of cellular materials. These theories are typically semi-empirical for PS, which retains its c-Si lattice structure in the solid skeleton around the pores, we show how the porosity dependence of the elastically can be incorporated into the representation of an anisotropic material. Many authors have made various efforts to explore thermodynamic properties of solids [1-5]. In these studies, the authors have examined the thermodynamic properties such as the inter-atomic separation and the bulk modulus of solids with

different approximation and best-fit relations. It has become possible to compute with great accuracy an important number of structural and electronic properties of solids. The abolition calculations are complex and require significant effort. Therefore, more empirical approaches have been developed [6,7] to compute properties of materials. In many cases, the empirical methods offer the advantage of applicability to a broad class of materials and to illustrate trends. In many applications, these empirical approaches do not give highly accurate results for each specific material, but are still very useful.

Cohen [8] has established an empirical formula for calculation of the bulk modulus B ; based on the nearest-neighbor distance. His result is in agreement with experimental values. Lam et al. [9] have derived an analytical expression for the bulk modulus from the total energy. This expression is different in structure from the empirical formula, but gives similar numerical results. Also, they have obtained an analytical expression for the pressure derivative B of the bulk modulus. The theory yields a formula with two attractive features. Only the lattice constant is required as input, the computation of B itself is trivial. Consideration of hypothetical structure and simulation of the experimental conditions is required to make practical use of this formula.

The aim is to see how a qualitative concept, such as the bulk modulus, shear modulus, young's modulus and plane modulus can be related to the energy gap and porosity of PS. It was argued that the dominant effect is the degree of covalency characterized by Phillips homopolar gap E_h [6], and one reason for presenting these data in this work is that the validity of the calculations that is not restricted in computed space.

The bulk modulus (B) for both bulk Si and PS is calculated using the Al-Douri et al relation:

$$B = (30 + 10 \lambda) \left(\frac{P}{E_{g\Gamma-X}^t} \right)^{1/4} / 3 \quad (1)$$

where P_t is the transition pressure, $E_{g\Gamma-X}$ is the energy gap along Γ -X and k is a parameter appropriate for the group-IV = 0, III-V = 1 and II-VI = 5 semiconductors.

Elastic materials exhibit a proportional relationship between an applied stress and the resulting tensile strain. The resulting linear relationship is known as Hooke's Law [7]. There are several ways available for calculating elastic constant of a method. The direct or traditional method is to apply a tension on the sample and calculate the corresponding strain and elastic constants from the tension-strain relationship. The traditional method is inconvenient, because for the calculations of all elastic constants several tensions need to be applied at several times.

The elastic constants of PS have been studied by measurement of the porosity on PS samples and its equation can be written as

$$C_{ij} = C_{ij}^0 (1 - P)^m \text{ where } m = 2.3 \quad (2)$$

If all the stiffness constants have this form of dependence of porosity, then the compliances S_{ij} all vary with the porosities as

$$S_{ij} = S_{ij}^0 (1 - P)^{-m} \quad (3)$$

here, C_{ij} are stiffness constants of the crystal and S_{ij} are the compliances of the crystal. For anisotropic cubic solids, the ratio $\eta = 2C_{44}/(C_{11}-C_{12})$ is commonly defined anisotropy factor [10].

2. RESULT AND DISCUSSION

2.1 Elastic Properties

Elastic properties are found to correlate well with strength and hardness in many materials. One of the important parameters that characterizes the physical property of a material system is bulk modulus which measures the degree of stiffness. The bulk modulus reflects important bonding characters in the material and, for many applications, is used as an indicator for material strength and hardness. Fig.1 displays bulk modulus (B) versus porosity (P) of PS samples for different current densities. By comparing the calculated results of 'B' with Bulk Si, the values are lower for all the PS samples. It is noticed from the figure that the values of 'B' decrease in the range 73.887 to 42.912 GPa as increase the porosity of PS upto 100 mA/cm². At 125 mA/cm², the 'B' slightly increases about 58.962 (GPa) and it again decreases to 50.361 (GPa) at 150 mA/cm².

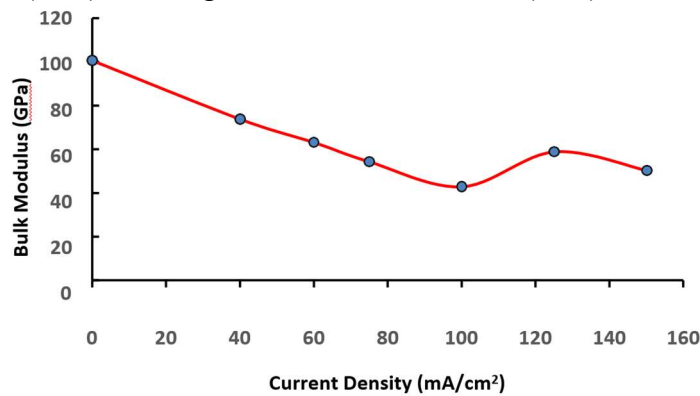


Fig. 1 Variation of bulk modulus with current density.

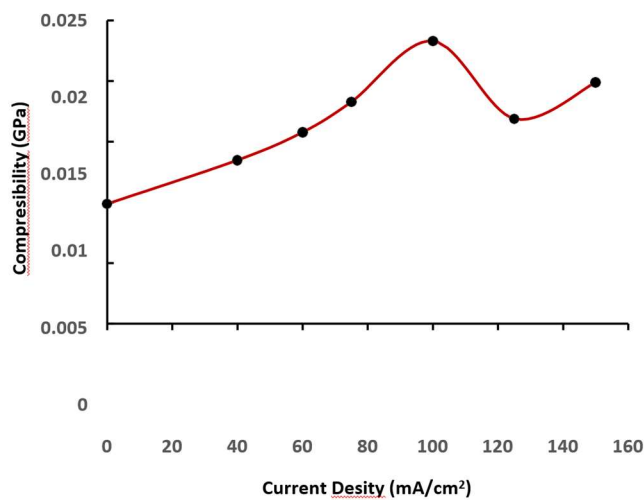


Fig. 2. Variation of compressibility with current density.

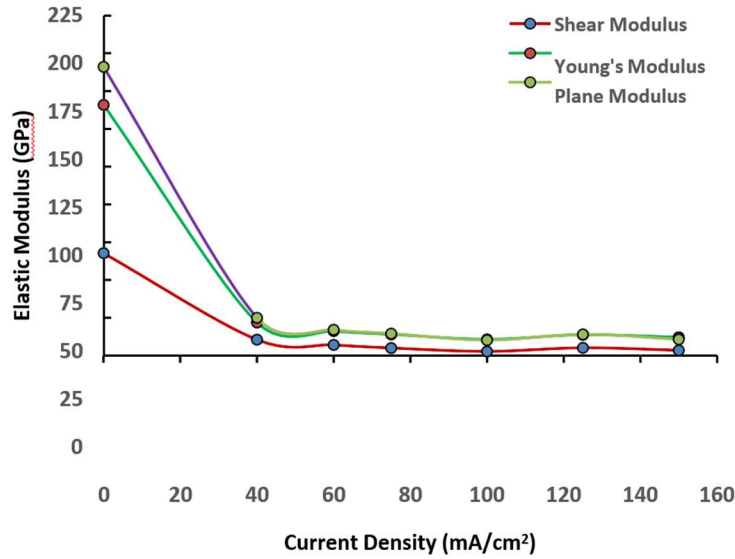


Fig. 3. Variation of elastic modulus with current density.

The reason for the change in sequence in ‘B’ at current density 125 mA/cm² is already given in the earlier section. The inverse of the bulk modulus gives a substance's compressibility (k). The decrease of ‘B’ suggests that PS becomes more compressible (Fig 2) with increasing current density, which in turn the percentage of porosity. The result concerning ‘B’ for bulk Si and PS is in good agreement with the experimental [11]. A similar trend is recorded in shear modulus (10.349 to 3.283 GPa), young’s modulus (21.701 to 11.936 GPa), Poisson ratio (0.3918 to 0.5978) and plane modulus (24.838 to 10.517) as a function of current density. The calculated results agree well with earlier reports [222,223]. As can be seen in the Fig. 4 the results concerning stiffness constants C11, C12, and C44 are decreased while the values of compliance S11, S12 and S44 increase with current density in the PS samples. The result of Bulk Si agrees reasonably well with those reported in the literature.

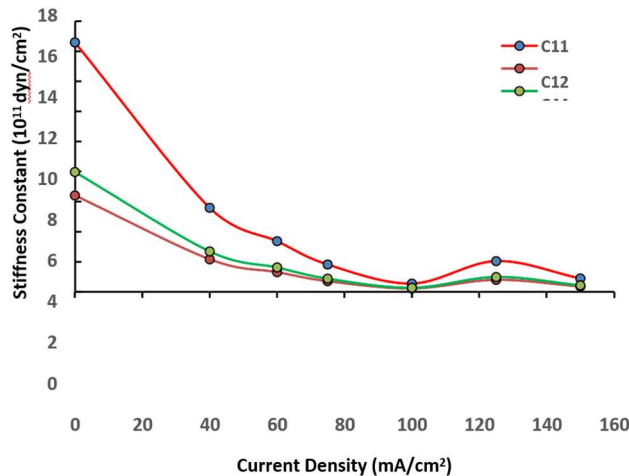


Fig. 4. Variation of stiffness constant with current density.

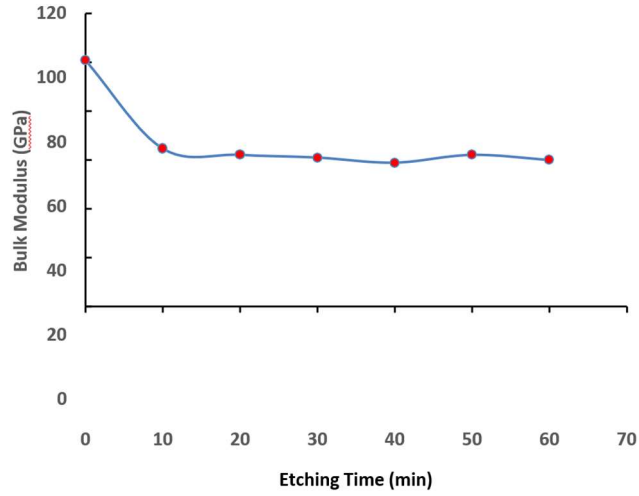


Fig. 5. Variation of bulk modulus with etching time.

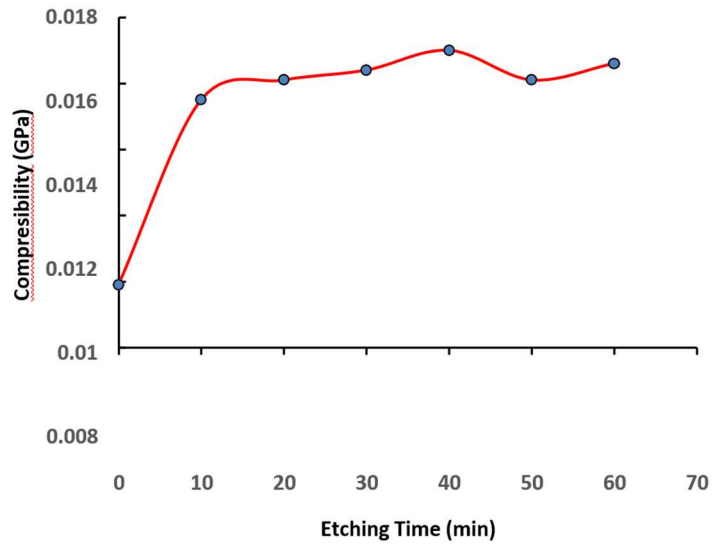


Fig. 6. Variation of compressibility in etching time.

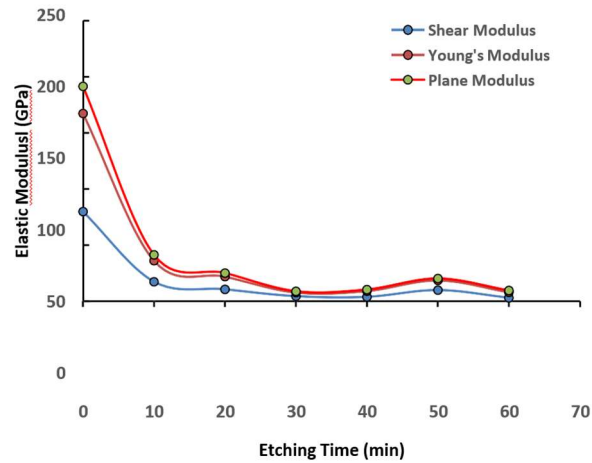


Fig. 7. Variation of elastic modulus with etching time.

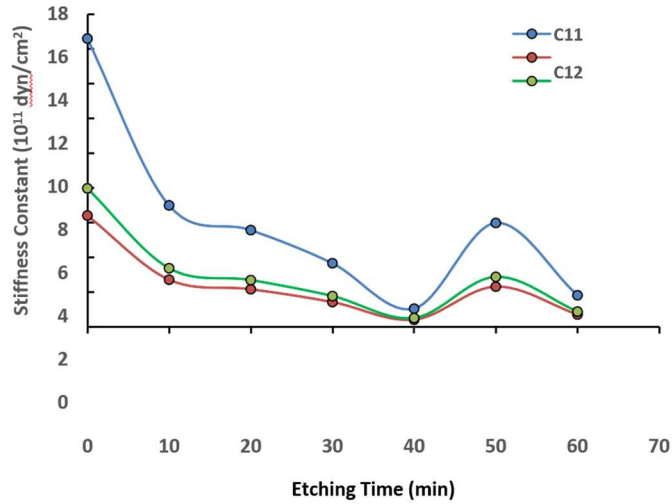


Fig. 8. Variation of stiffness constant with etching time.

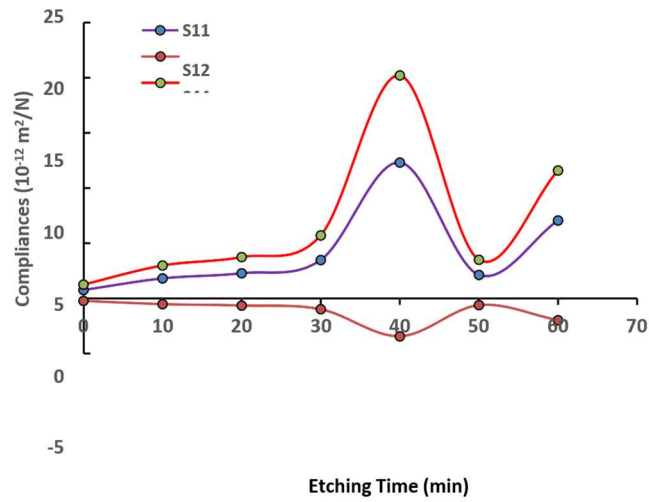


Fig. 9. Variation of compliances constant with etching time.

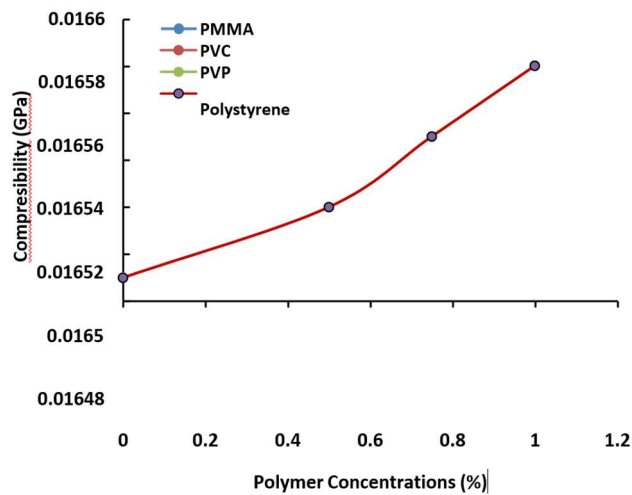


Fig. 10. Variation of compressibility with polymer concentrations.

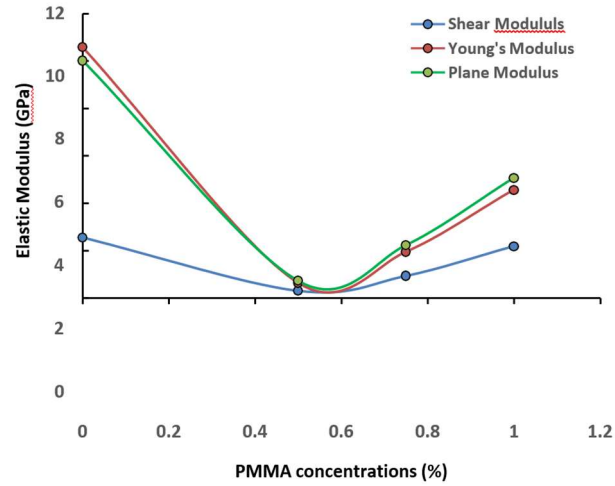


Fig. 11. Variation of elastic modulus with PMMA concentrations.

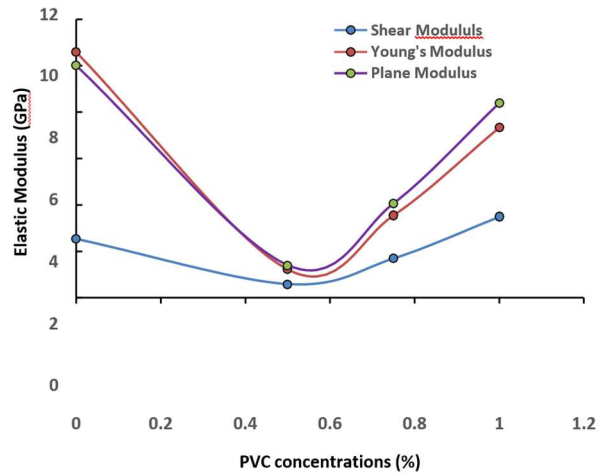


Fig. 12. Variation of elastic modulus with PVC concentrations.

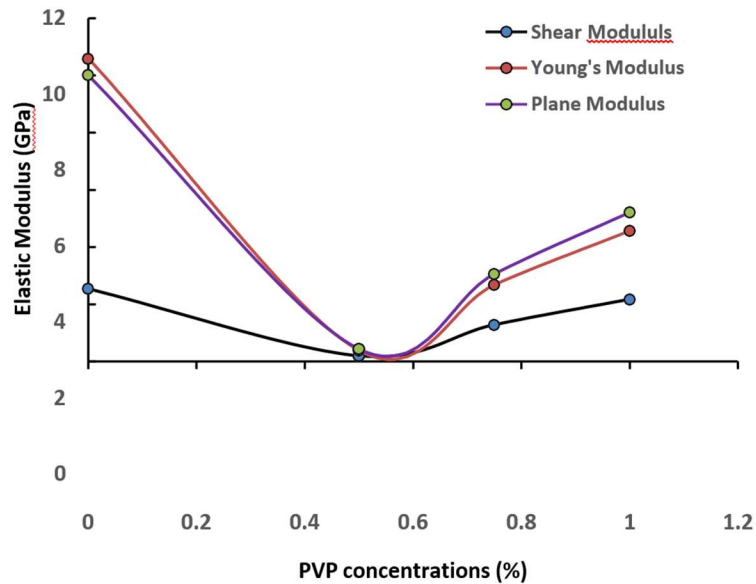


Fig. 13. Variation of elastic modulus with PVP concentrations.

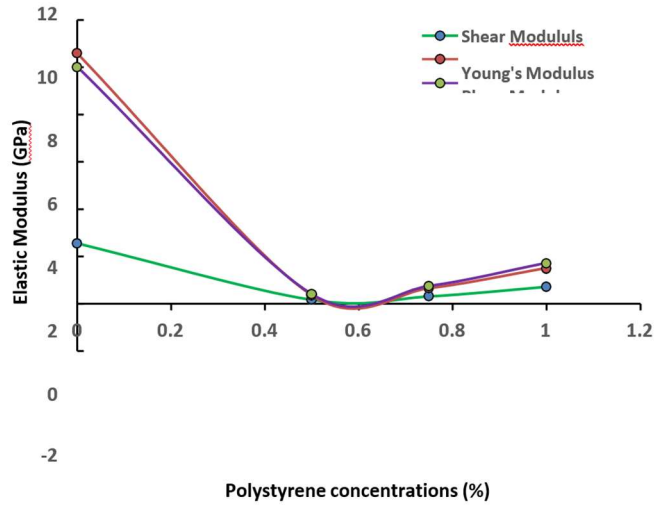


Fig. 14. Variation of elastic modulus with Polystyrene concentrations.

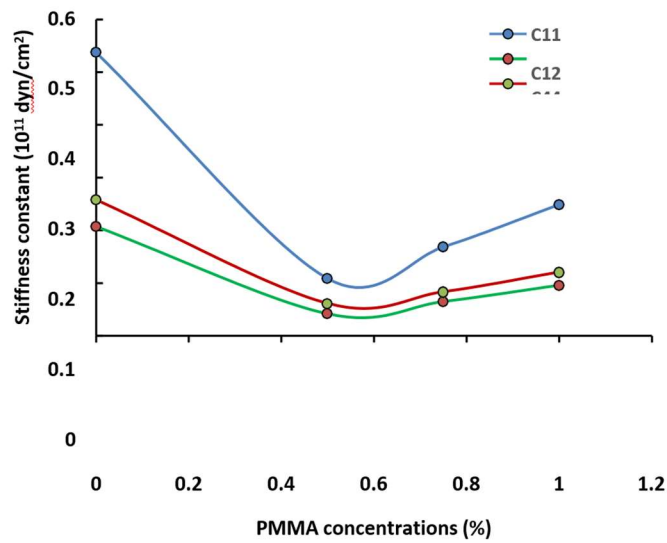


Fig. 15. Variation of stiffness constant with PMMA concentrations.

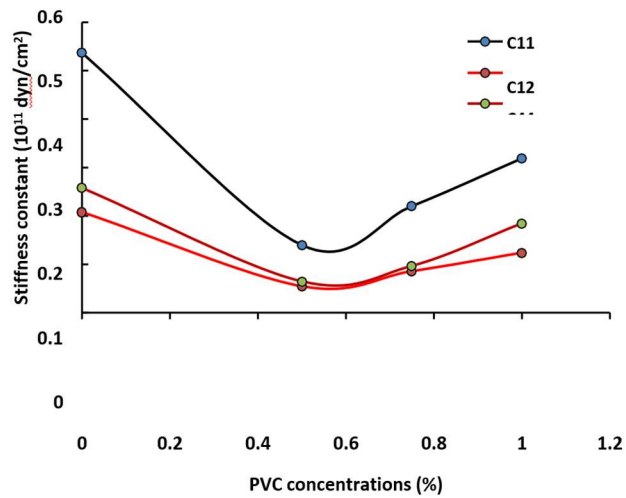


Fig. 16. Variation of stiffness constant with PVC concentrations.

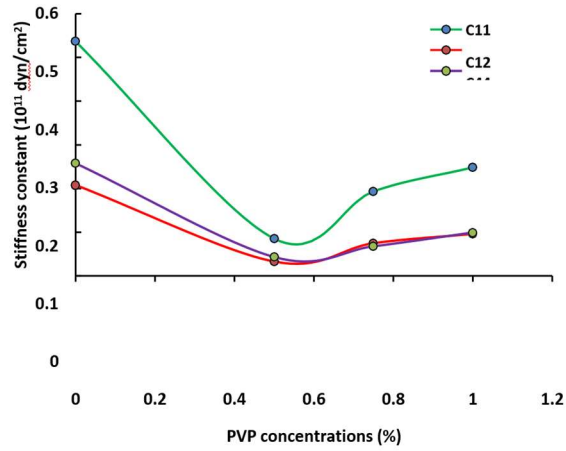


Fig. 17. Variation of stiffness constant with PVP concentrations.

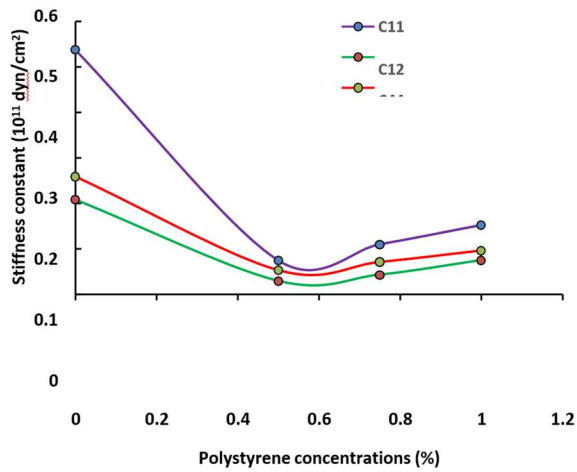


Fig. 18. Variation of stiffness constant with Polystyrene concentrations.

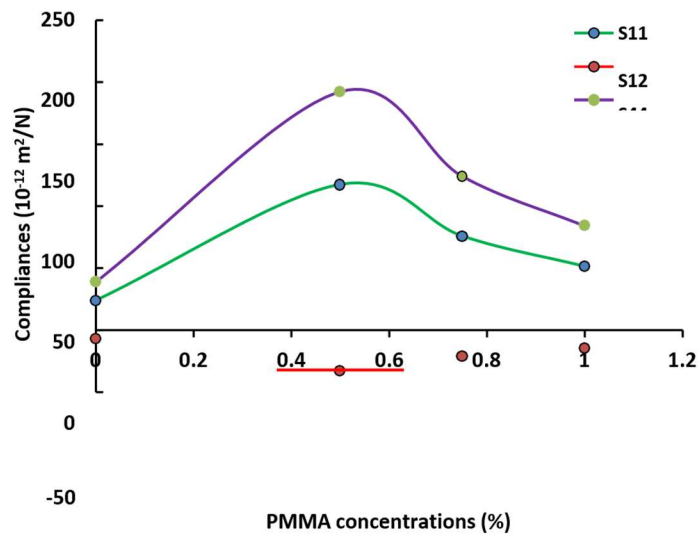


Fig. 19. Variation of compliances with PMMA concentrations.

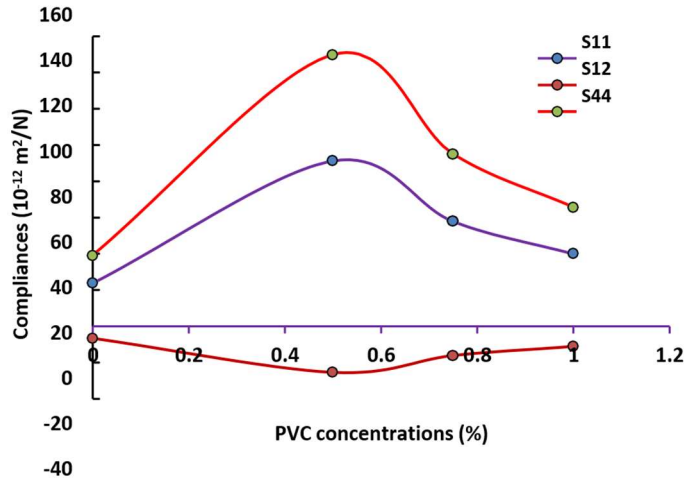


Fig. 20. Variation of compliances with PVC concentrations.

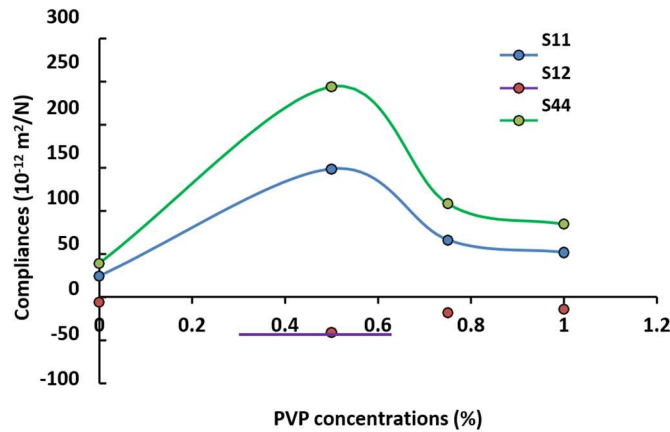


Fig. 21. Variation of compliances with PVP concentrations.

In the case of PS, the calculated values of stiffness and compliances are related to the percentage of porosity of PS. In summary, the calculated stiffness constant for different current density are found in the range of 5.5707 to 0.8760 for C11, 2.1495 to 0.3380 for C12 and 2.6743 to 0.4205 for C44. While the compliances are found in the range of 2.2829 to 14.5179 for S11, -0.6361 to -4.0453 for S12 and 3.7455 to 23.8185 for S44. The results of elastic constant are reflected the percentage of porosity of PS and the method proves as a suitable way to determine the relationship between an applied stress and the resulting tensile strain. Interestingly, the calculated anisotropic constant of the both Bulk Si and PS samples are found to be around 1.560 indicating the systems are anisotropic nature. Note that the ‘ η ’ is 1 commonly for isotropic solid. The results can be correlated with SEM images (anisotropic) for different current densities. SEM images contain heterogeneous pores, and polygonal c-Si grains. The elastic properties of PS fabricated with different etching time (at 100mA/cm² for 30 min) illustrated in Fig. (5-9) respectively. By comparing the figures that the elastic properties such as B, K, G, E, γ and M of PS with different etching time seems to similar sequence to that of PS with different current densities. Although the calculated values are slightly lower in PS with different etching time. It briefly, the elastic

parameters decrease except compressibility (K) with the percentage of porosities, up to 40 min etching and it slightly increases at 50 min etching. While these parameters again increased at 60 min etching time. The noticeable change in sequence in etching time between 50 – 60 min is due to pore formation occurring in the next layer of c-Si wafer as visually evidenced by SEM results. The results of elastic constant (stiffness and compliances) and anisotropy constant of PS are reflected as in the case PS samples fabricated with different current densities.

By comparing the elastic properties, elastic constants and anisotropic constants of polymers treated PS (Figs. 10-21) with PS samples (current densities and etching time), the calculated 'B' values decrease with increase the polymer concentrations. The values 'B' found in the range of 60.4964 – 60.3136 GPa and the values are close to the Bulk Si. The compressibility found to increase with increase the polymer concentration. The remaining elastic properties G , E , γ and M are found to be increase with polymer concentrations. While the stiffness constant increase whereas compliances are increased with polymer concentrations. The sequences are opposite to the effect of current densities and time of PS samples. The close scrutiny of the orientation changes is related to pore infiltration of the polymers lead to form a thin layer over the PS surface. As obviously visible in the SEM analysis. Besides, the pore infiltration is more in PVP and Polystyrene treated PS samples than PMMA and PVC treated samples. The same trend is found in the experimental studies also. It is concluded that the theoretical calculations are useful to correlate the experimental results.

3. CONCLUSION

In summary, this passage underscores the crucial role of elastic properties, particularly the bulk modulus (B), in evaluating material strength and hardness. The bulk modulus serves as a vital indicator of a material's stiffness and bonding characteristics. It is exemplified through a graphical representation (Fig. 1) of bulk modulus (B) against porosity (P) in polystyrene (PS) samples subjected to varying current densities. When comparing PS's calculated bulk modulus (B) with Bulk Silicon (Bulk Si), it becomes evident that PS exhibits lower bulk modulus values. As porosity increases up to a current density of 100 mA/cm², the bulk modulus (B) consistently decreases within the range of 73.887 to 42.912 GPa, signifying that increased porosity results in reduced stiffness. At 125 mA/cm², a slight increase in bulk modulus (B) to approximately 58.962 GPa indicates subtle changes in material properties. However, at a higher current density of 150 mA/cm², the bulk modulus (B) declines to 50.361 GPa, indicating decreased stiffness. These findings emphasize porosity's significant influence on bulk modulus and, consequently, the stiffness of PS, offering critical insights into material mechanical properties, especially in applications prioritizing strength and hardness.

In conclusion, the shift in bulk modulus (B) at a current density of 125 mA/cm² is attributed to the increased compressibility of polystyrene (PS) as porosity and current density rise, aligning with experimental results [11]. Similar trends are observed in other material properties such as shear modulus, Young's modulus, Poisson's ratio, and plane modulus, all of which decrease with rising current density, consistent with prior research [12,13]. Furthermore, stiffness constants C_{11} , C_{12} ,

and C44 decrease, while compliance values S11, S12, and S44 increase with current density in the PS samples, in reasonable agreement with reported data for Bulk Silicon. Stiffness constants (C11, C12, C44) for PS range from 5.5707 to 0.8760, and compliances (S11, S12, S44) span from 2.2829 to 14.5179, consistently decreasing with increasing porosity, except for compressibility (K), which slightly increases at specific etching times. Both Bulk Silicon and PS exhibit anisotropic behavior, with an anisotropic constant (η) of approximately 1.560, indicating their anisotropic nature, as supported by SEM images showing heterogeneous pores and polygonal c-Si grains. Elastic properties of PS treated with different etching times follow a similar sequence to those treated with different current densities, albeit with slightly lower calculated values. Notably, the change in sequence at specific etching times results from pore formation in the next layer of the c-Si wafer, observed in SEM results.

When comparing elastic properties of PS treated with polymers to PS samples influenced by current densities and etching time, contrasting trends emerge. 'B' values decrease with increasing polymer concentrations (60.4964 to 60.3136 GPa), approaching Bulk Si values. Compressibility increases with polymer concentration, while other elastic properties (G, E, γ , M) and stiffness constants increase, contrary to previous trends. These variations correlate with polymer pore infiltration, forming a thin layer on the PS surface, more pronounced in PVP and Polystyrene-treated PS samples compared to PMMA and PVC-treated samples, aligning with experimental studies. Theoretical calculations effectively complement experimental findings, providing comprehensive insights into how factors like porosity, current density, etching time, and polymer concentration influence PS's elastic properties. In summary, this research illuminates the intricate interplay between material properties and processing parameters, with potential implications for various applications involving porous materials like PS.

4. REFERENCES

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