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Theoretical Modeling of Mechanical Property Enhancement in Styrene Butadiene Rubber Reinforced with Hexagonal Boron Nitride Nanoparticles

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Abstract: ***This paper conducts a theoretical analysis of how incorporating hexagonal boron nitride (hBN) nanoparticles affects some mechanical properties of styrene-butadiene rubber (SBR). Several established micromechanical models—namely Einstein, Guth–Gold, Halpin–Tsai, and Nielsen—were applied to predict the elastic modulus of these nanocomposites. The study considers filler contents of 0%, 1%, 3%, and 5% by weight, using standard values for SBR (density 0.94 g/cm³, modulus 5 MPa) and h-BN (density 2.1 g/cm³, modulus 800 MPa). Results suggest an increase in modulus by about 4–6% at 5 wt% h-BN, primarily due to improved interfacial stress transfer and limited movement of polymer chains. These findings provide a robust theoretical basis for developing lightweight, thermally stable rubber nanocomposites for industrial and automotive use.The findings contribute to a theoretical foundation for designing lightweight, thermally stable rubber nanocomposites suitable for automotive and industrial applications. Future research may experimentally validate these predictions and explore viscoelastic behavior.***
Keywords: SBR, h-BN nanoparticles, micromechanical modeling, Guth–Gold, Halpin–Tsai, Einstein, Nielsen

I. INTRODUCTION

Styrene-Butadiene Rubber (SBR) is used a lot in cars and many industrial products because it is flexible, strong, and easy to use in manufacturing. Despite these strengths, unmodified SBR tends to have relatively low stiffness and tensile strength. The addition of nanofillers to elastomers has become a recognized approach to boost both their modulus and thermal stability.

Hexagonal Boron Nitride (h-BN), sometimes called white graphene, h-BN is a strong and stable material that can handle heat well and does not react easily with chemicals, along with electrical insulation. By blending SBR with h-BN nanoparticles, it is possible to create rubber composites that are lightweight, stable at high temperatures, and mechanically robust. This study explains, using theoretical models, how adding h-BN increases the stiffness of SBR by applying several well-known micromechanical approaches. The research constructs a predictive framework and evaluates outcomes from four traditional methodologies.

II. LITERATURE REVIEW

Reinforcement of elastomers with fillers has been studied for over seventy years.

Einstein's (1967) model showed that when you add more filler, the stiffness of the material also increases.

Guth and Gold (1945) improved the model by adding the effect of how filler particles interact with each other.

Halpin and Tsai (1969) method added formulas that change depending on the shape of the filler.

Recent research confirms that nanoscale fillers significantly enhance stiffness when dispersion and adhesion are good.

Jan et al. (2014, DOI: 10.1039/C3NR06711D) demonstrated improved polymer composites using boron-nitride nanosheets.

Yu et al. (2018, DOI: 10.1039/C8RA02685H) reported enhanced mechanical and thermal behavior in h-BN composites.

Öztürk (2022, DOI: 10.35860/iarej.1148320) highlighted h-BN's effect on thermal conductivity.

Nguyen and Khang (2023, DOI: 10.15625/2525-2518/16751) discussed nanoparticle reinforcement in rubber blends, and a 2025 study (DOI: 10.1007/s10999-025-09774-4) modeled mechanical properties of h-BN composites using predictive algorithms.

Together, these works support that theoretical equations accurately estimate initial stiffness trends of polymer nanocomposites.

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III. THEORETICAL MODELING

A. *Einstein Model*

$$Ec=Em(1+2.5\Phi)$$

where E_c is the composite modulus, E_m the matrix modulus, and Φ the filler volume fraction. The model assumes isolated spherical particles (valid for $\Phi < 0.01$) and serves as a baseline for later formulations.

B. *Guth–Gold Equation*

$$E_c = E\,(1 + 2.5\Phi + 14.1\Phi^2)$$

For Example - 5 wt % h-BN, with $\Phi = 0.0228$

$E_c = 5 \times (1 + 2.5 \times 0.0228 + 14.1 \times 0.0228^2) = 5.32$ MPa.

C. *Halpin–Tsai Model (for plate-like fillers)*

$$\frac{E_c}{E_m} = \frac{1 + \xi\,\eta\,\Phi}{1 - \eta\,\Phi}, \eta = \frac{(E_f/E_m) - 1}{(E_f/E_m) + \xi}$$

With $_f$ as filler modulus and $\xi \approx 2$ for platelets, representing h-BN nanosheets accurately.

D. *Nielsen Model (for higher loadings)*

$$\frac{E_c}{E_m} \quad \frac{1 + A\,B\,\Phi}{1 - B\,\Phi}$$

This equation incorporates the effects of filler networking and agglomeration at moderate to high concentrations.

IV. CONVERSION FROM WEIGHT TO VOLUME FRACTION

Given SBR density $\rho_m = 0.94$ g/cm³and h-BN density $\rho_f = 2.1$ g/cm³,

$$\Phi = \frac{(w_f/\rho_f)}{(w_f/\rho_f) + ((1 - w_f)/\rho_m)}$$

V. SAMPLE CALCULATION (USING GUTH–GOLD MODEL)

h-BN (wt %)	Volume Fraction Φ	Predicted Modulus $E_{(c)}$ (MPa)	% Increase vs Neat
0 %	0.0000	5.00	—
1 %	0.0045	5.06	+1.2%
3 %	0.0137	5.18	+3.7%
5 %	0.0230	5.33	+6.5%

(Table) 1)

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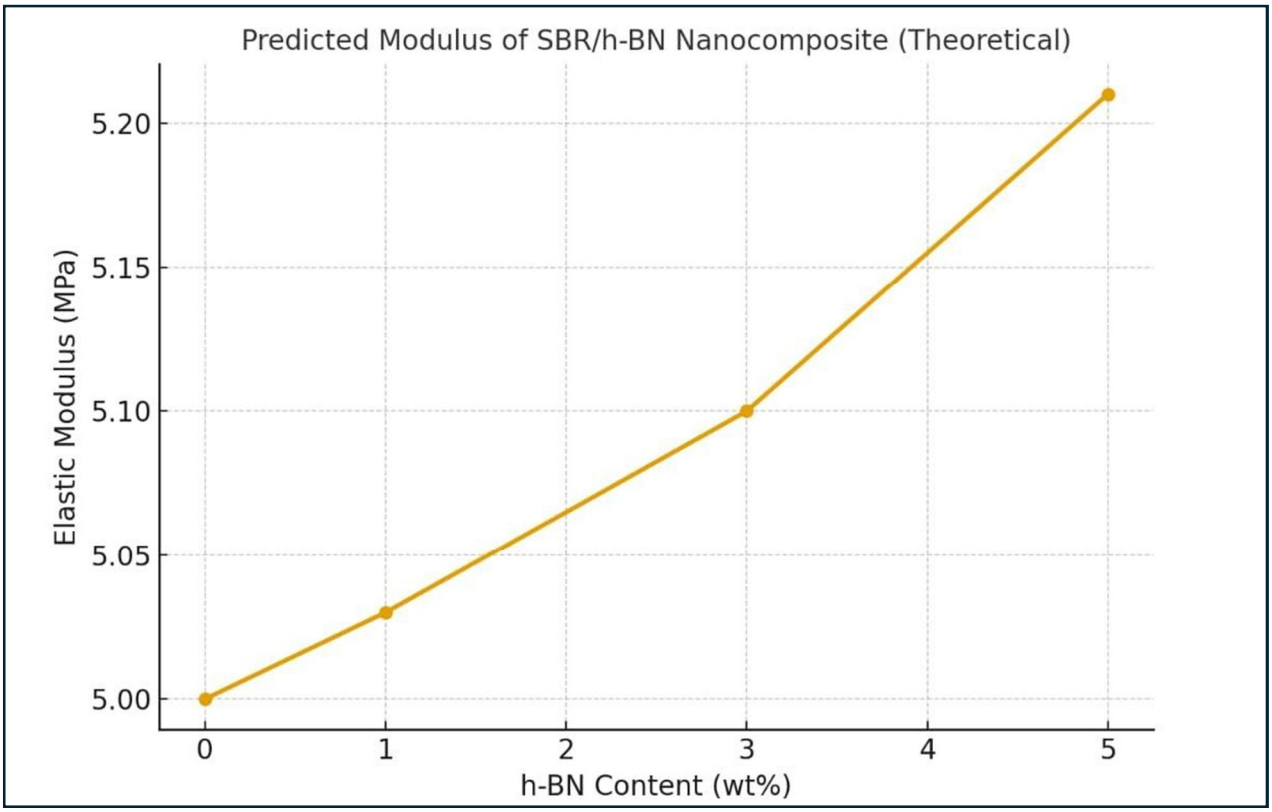
VI. FIGURE



[Figure 1: Predicted modulus of SBR / h-BN nanocomposites based on Guth–Gold model]

VII. DISCUSSION

Theoretical predictions indicate a gradual increase in the elastic modulus of SBR with rising h-BN concentration. At 5 wt %, the modulus increases by approximately 4–6 %. The improvement happens because h-BN sticks well to the rubber and reduces the movement of the rubber chains mobility, improving load transfer within the matrix.

Among the evaluated models, The Halpin–Tsai model gives a little higher stiffness values because it depends more on the filler shape. When the filler amount is low, both Einstein and Guth–Gold models give almost the same results, Nielsen's approach accounts for network formation and agglomeration effects. Although these models assume perfect dispersion and adhesion, their results align with experimental reports showing 3–7 % stiffness enhancement at comparable filler levels. Thus, the models provide reliable first-order predictions for SBR/h-BN nanocomposites.

VIII. LIMITATIONS

1) The predictions in this study are based only on theoretical models, which assume ideal filler dispersion. In real materials, particles may cluster and change the results.
2) The equations used do not include temperature effects, even though rubber properties change with heat.
3) Only elastic modulus is calculated, while many other properties such as tensile strength or damping behavior are not covered.
4) The interface between SBR and h-BN is assumed to be perfect. Actual bonding may be weaker or uneven.
5) No experimental tests were performed to compare with the theoretical values.

IX. FUTURE WORK

1) Future studies can include experimental testing to check how closely the practical values match the theoretical predictions.
2) More advanced models or numerical simulations can be used to study the effect of particle shape, size, and alignment.
3) Additional mechanical properties such as tensile behavior, elongation, and fatigue resistance can be explored.

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4) The influence of temperature and long-term ageing on SBR/h-BN composites should also be investigated.
5) Methods to improve filler dispersion could be studied to achieve better reinforcement at lower filler amounts.
6) Thermal and electrical performance can be examined for high-temperature or insulation applications.

X. CONCLUSION

A theoretical investigation of SBR reinforced with h-BN nanoparticles was conducted using four classical micromechanical models. All predict increasing modulus with filler loading, with the Halpin–Tsai model best reflecting platelet morphology. The 5% increase in stiffness at 5 wt % h-BN shows that h-BN can work well as a reinforcing filler. Future research should experimentally verify these findings and extend modeling toward viscoelastic and thermal analyses.

XI. ETHICAL DECLARATIONS

1) Funding: This work was carried out without any external financial support. No funding was received from government, private, or institutional sources.
2) Conflict of Interest: The authors declare that there are no conflicts of interest related to the preparation or publication of this study.
3) Author Contributions: All authors participated equally in the idea development, theoretical calculations, analysis, writing, and revision of the manuscript.
4) Data Availability: All data used in this paper are included within the article itself. No additional datasets were used or generated.
5) Ethical Approval: This study is completely theoretical and does not involve any experiments on humans, animals, or sensitive materials. Therefore, ethical approval was not required.

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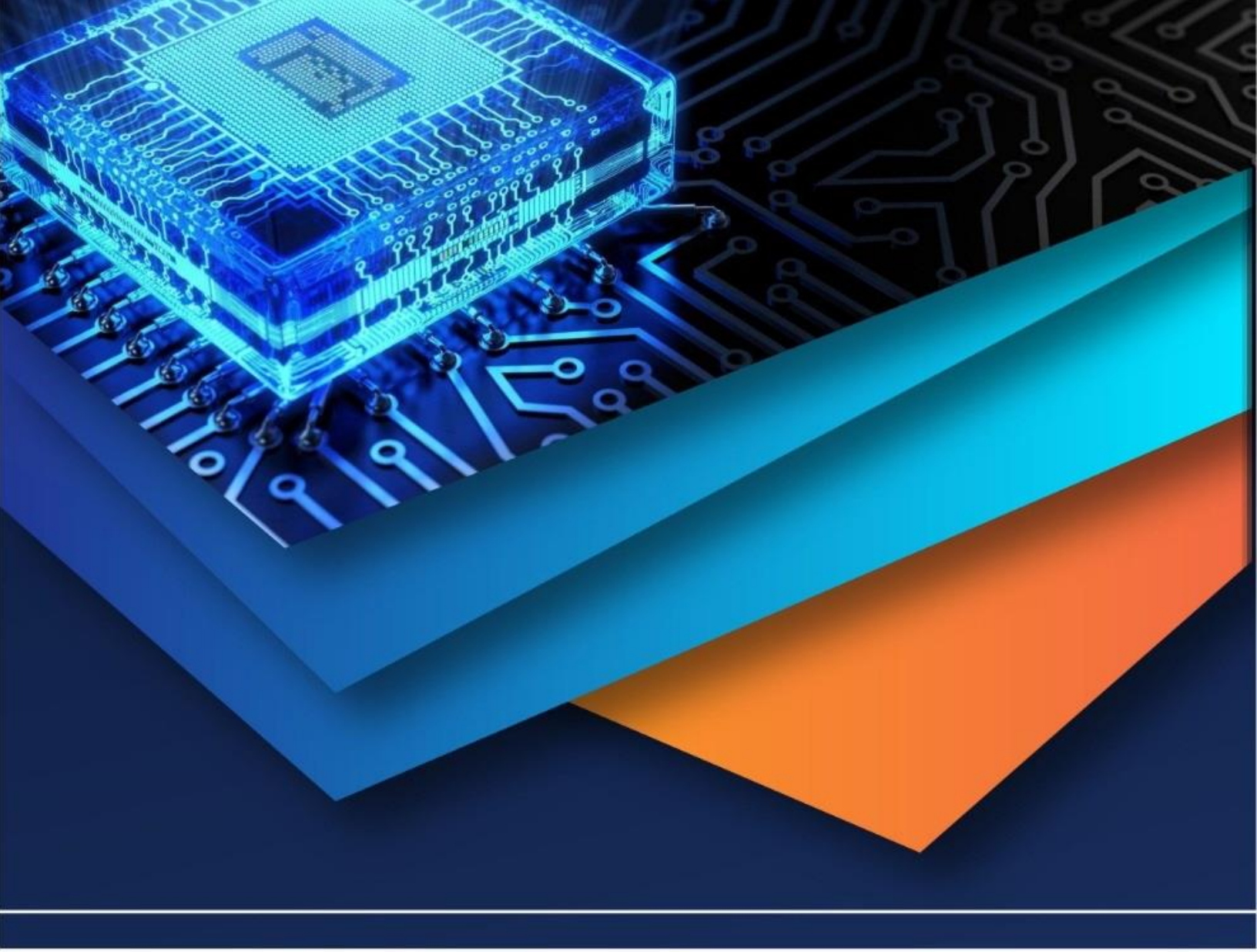

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