BN-Defect Engineering in TPH-Graphene Mechanics

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1. Introduction

TPH-graphene exhibits outstanding mechanical properties that can be tuned through chemical doping [1]. Here, we investigate the effect of progressively substituting carbon atoms with boron–nitrogen pairs in a TPH-graphene monolayer, generating a family of seven BN-engineered structures ranging from the pristine system to higher BN contents. For each configuration, we assess the mechanical response under uniaxial loading by evaluating Young's modulus and the Von Mises stress distribution over the 100–700 K temperature range. This analysis elucidates how BN substitution and temperature jointly govern the mechanical behavior of TPH-graphene, providing guidance for designing two-dimensional nanomaterials with controllable, application-specific properties.

2. Computational Details

All calculations were performed using classical molecular dynamics simulations implemented in LAMMPS [2]. Simulations were carried out on two-dimensional TPH-graphene monolayers and their boron–nitrogen–doped variants, with lateral dimensions of approximately 100 Å × 100 Å. The structures were first equilibrated at temperatures between 100 and 700 K using an NPT ensemble, with pressure control applied along the loading direction. Subsequently, quasi-static uniaxial tensile strain was applied along the x axis while maintaining periodic boundary conditions in the plane. Interatomic interactions were described using a Tersoff-type potential, which is well suited to capture the bond-order–dependent response of covalent networks under deformation [3]. From the resulting stress–strain curves, Young's modulus and the Von Mises stress distribution were computed, enabling assessment of the combined effects of BN substitution and temperature on the mechanical properties of the material.

5. Conclusions

The incorporation of BN pairs consistently reduces Young's modulus across the entire temperature range (100–700 K) for uniaxial loading along both the X and Y directions, indicating an overall stiffness degradation relative to pristine TPH-gr. In addition, BN substitution disrupts the characteristic stress-transfer pathways observed in TPH-gr, leading to a modified spatial distribution of the Von Mises stress.
Despite the reduction in elastic stiffness, BN pairs promote a more favorable mechanical response in the plastic regime by redistributing local stress concentrations, which enhances deformation accommodation after yielding compared with the pristine monolayer.

6. References

[1] J. Li, et al., J. Phys. Chem. Lett., vol. 12, no. 2, pp. 732–738, 2021.
[2] A. P. Thompson et al., Comput. Phys. Commun., vol. 271, p. 108171, 2022.
[3] J. Tersoff, Phys. Rev. B, vol. 37, no. 12, pp. 6991-7000, 1988.

3. Results

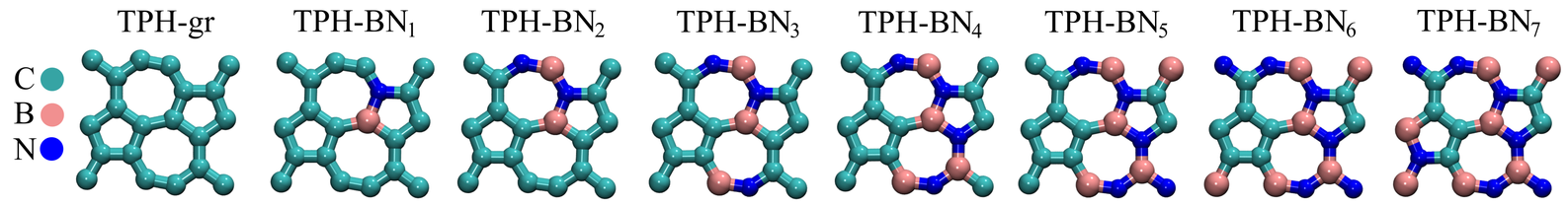

Figure 1. Atomic models of the studied TPH-graphene monolayers, from pristine TPH-gr to BN-defect–engineered TPH-BN_7, generated by the progressive substitution of C atoms with BN pairs (1–7 pairs).

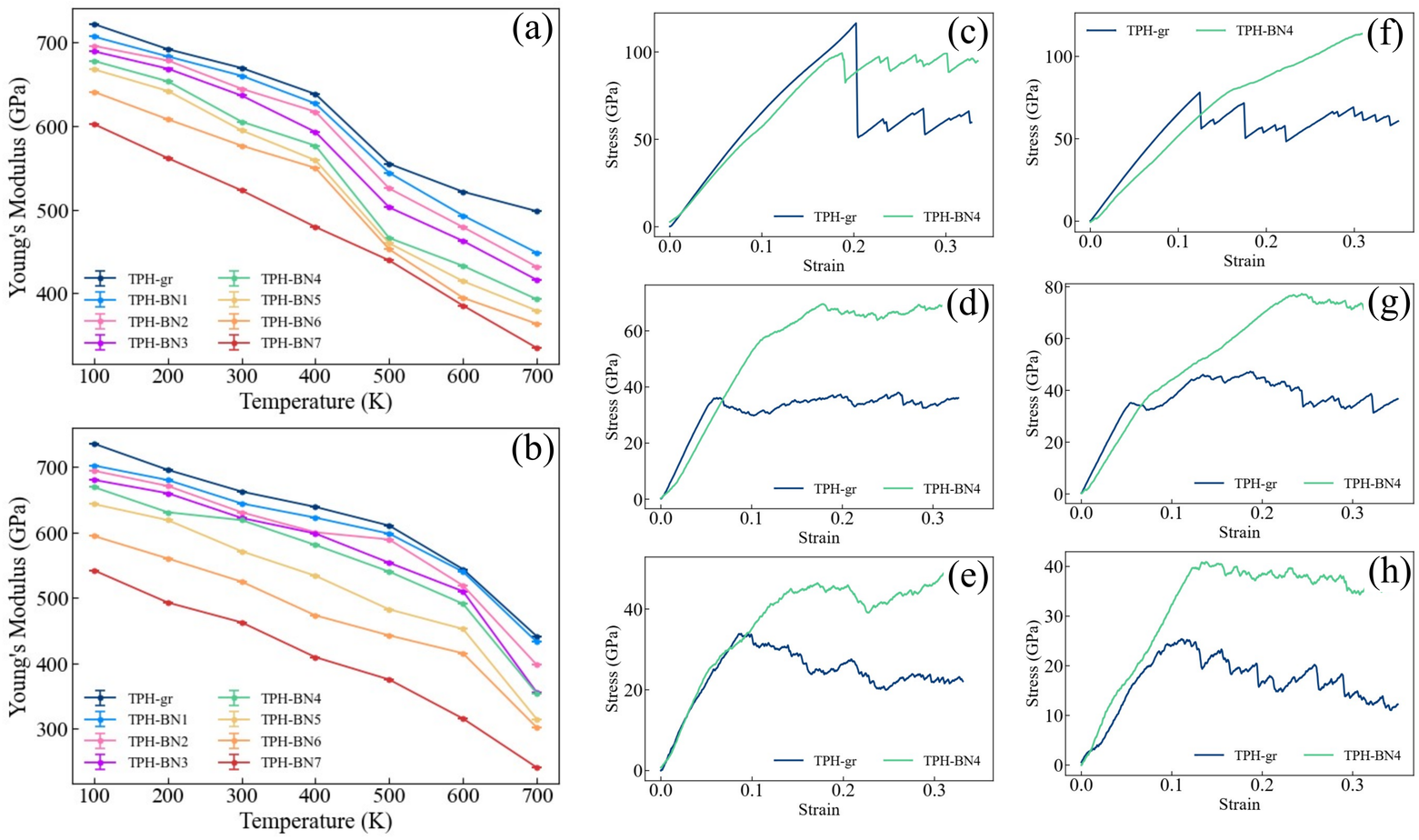

Figure 2. Temperature dependence of Young's modulus for TPH-gr and BN-defected TPH-BN_n (n = 1-7) under uniaxial loading along (a) X and (b) Y. Representative stress-strain responses of TPH-gr and TPH-BN_4 at (c,f) 100 K, (d,g) 400 K, and (e,h) 700 K for deformation applied along X (c–e) and along Y (f–h), respectively.

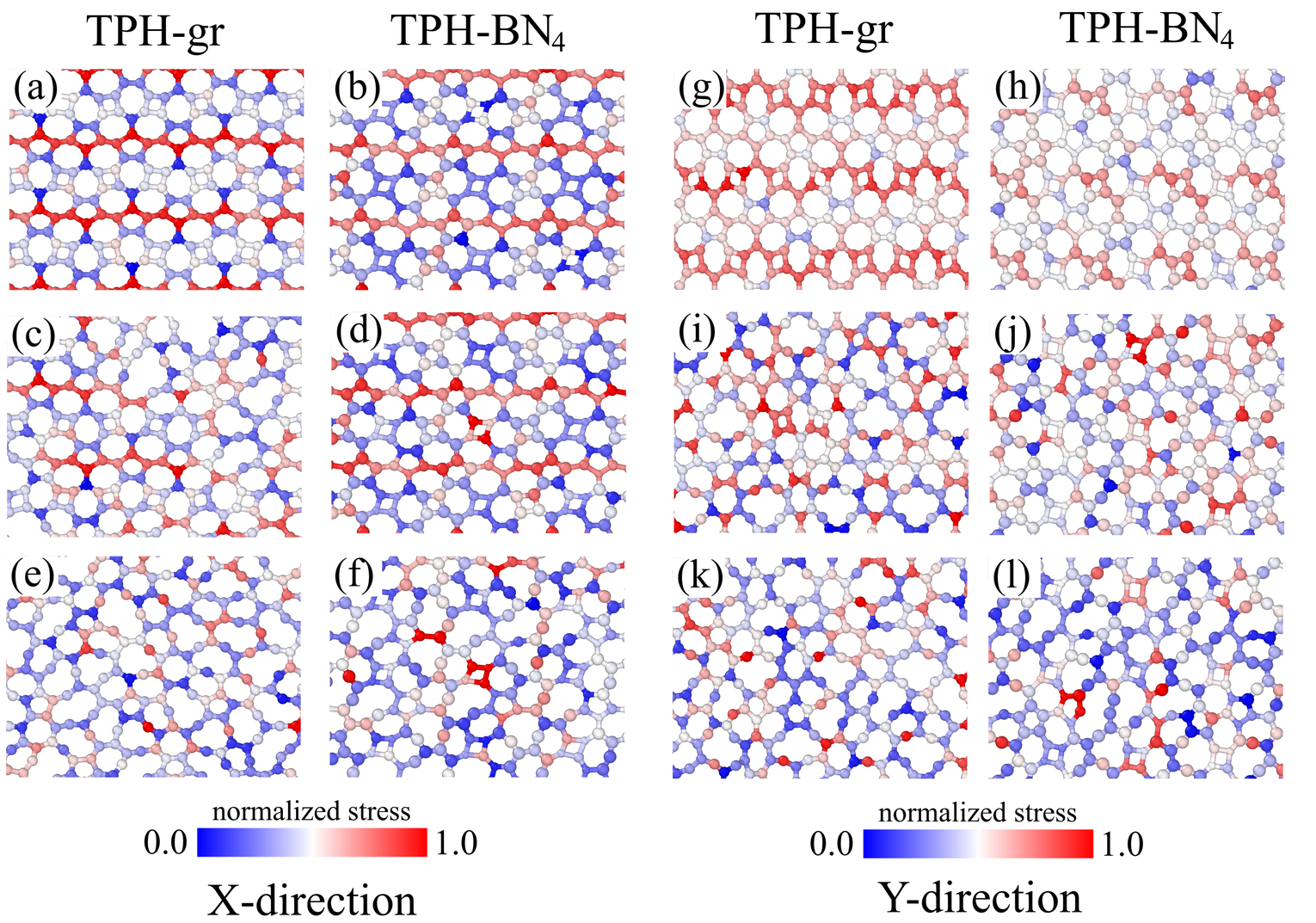

Figure 3. Von Mises stress distributions at 10% strain for TPH-gr and TPH-BN_4 under uniaxial deformation along X at 100 K, 400 K, and 700 K: (a,c,e) TPH-gr and (b,d,f) TPH-BN_4. Corresponding maps at 10% strain for deformation along Y at 100 K, 400 K, and 700 K: (g,i,k) TPH-gr and (h,j,l) TPH-BN_4.