

# Mechanical and Tribological Properties of Nitrile Rubber Reinforced by SiO<sub>2</sub>: Molecular Dynamics Simulation

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### Research Article

**Keywords:** mechanical and tribological properties, nitrile rubber, molecular dynamics simulation, nano-SiO<sub>2</sub>

**Posted Date:** March 11th, 2021

**DOI:** <https://doi.org/10.21203/rs.3.rs-194024/v1>

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**Version of Record:** A version of this preprint was published at Tribology Letters on April 9th, 2021. See the published version at <https://doi.org/10.1007/s11249-021-01427-9>.

# Abstract

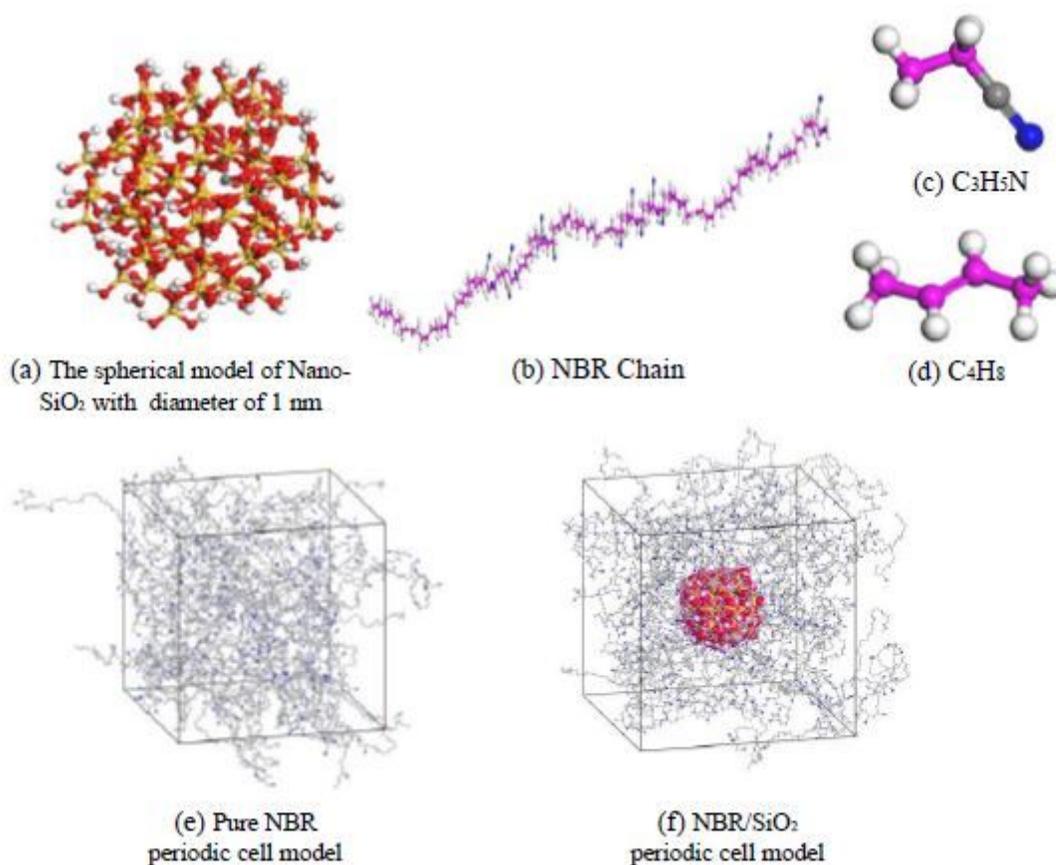
This paper investigated the mechanism of enhancing the mechanical and tribological properties of nitrile rubber (NBR) with SiO<sub>2</sub> on the molecular scale. Molecular dynamics (MD) simulations were performed on molecular structure models of pure NBR, NBR/SiO<sub>2</sub> and three-layer friction pairs. The results showed that the hydrogen bonds and interfacial interaction between SiO<sub>2</sub> and NBR molecular chains decreased the fractional free volume of NBR nanocomposites, and increased the shear modulus of NBR by 25% compared with that of pure NBR. During the friction process, SiO<sub>2</sub> decreased the radius of gyration of NBR molecular chains and effectively lowered the peak atomic velocity, the peak temperature and the peak friction stress at the interface between NBR and copper atoms. The average friction stress on NBR/SiO<sub>2</sub> was 34% lower than that on NBR, which meant the tribological properties of NBR were significantly improved by SiO<sub>2</sub>. The mechanism of SiO<sub>2</sub> reinforcing NBR on a molecular scale can lay a theoretical foundation for the design of water-lubricated rubber bearings.

# Full Text

Due to technical limitations, full-text HTML conversion of this manuscript could not be completed. However, the latest manuscript can be downloaded and [accessed as a PDF](#).

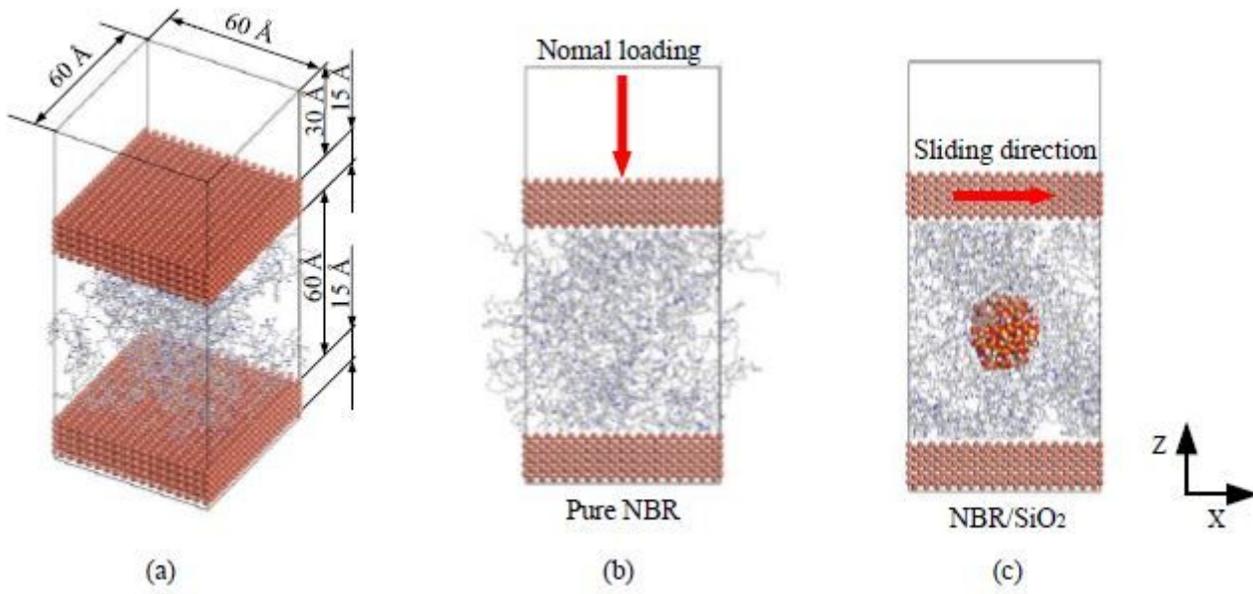
# Figures

- H
- O
- N
- C
- Cu
- Si



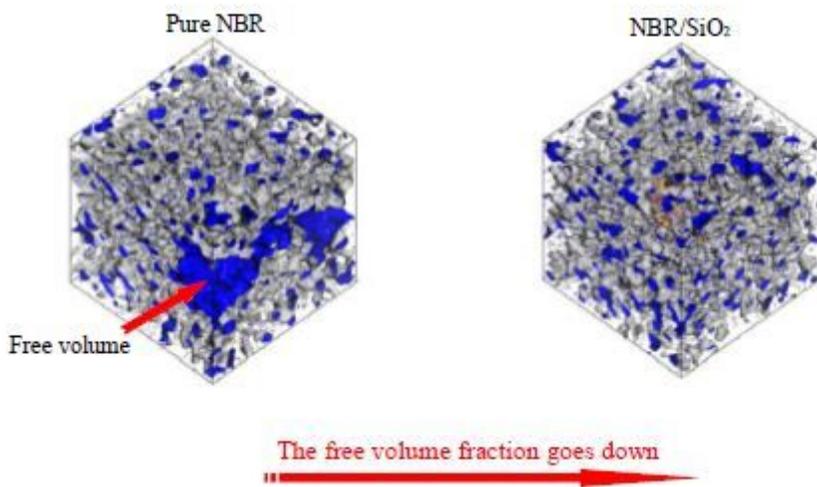
**Figure 1**

The structural model of NBR filled with nano-SiO<sub>2</sub> (SiO<sub>2</sub> (TESPT))



**Figure 2**

Three-layer molecular models for shear friction pairs



**Figure 3**

Free volume of pure NBR and NBR/SiO<sub>2</sub>

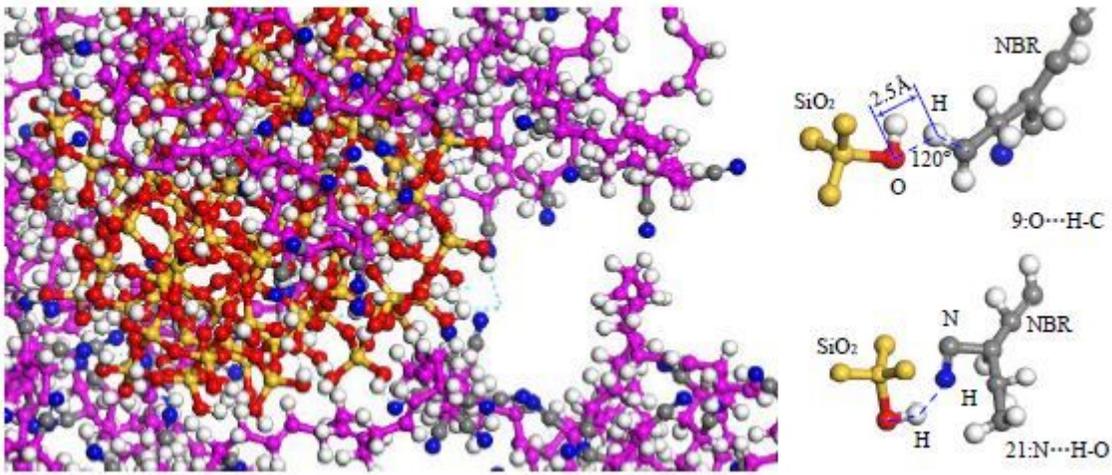


Figure 4

The hydrogen bonds formed between nano-SiO<sub>2</sub> and NBR

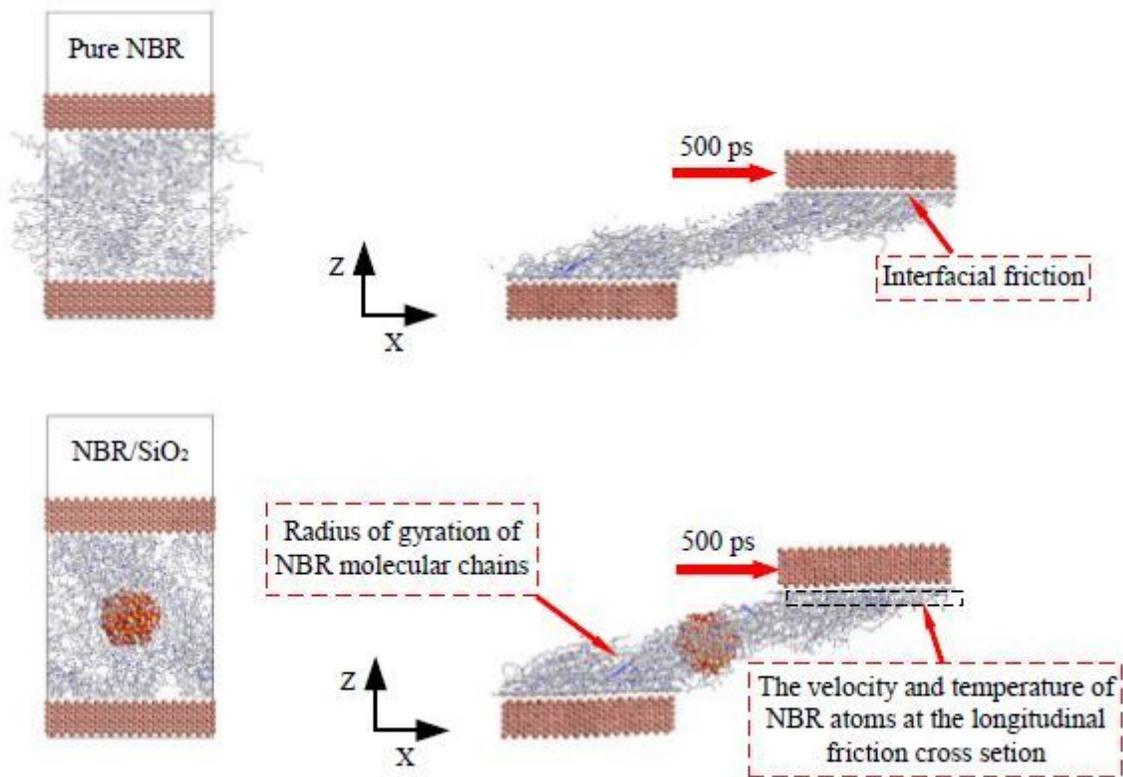


Figure 5

Pictures of shear friction simulation for pure NBR and NBR/SiO<sub>2</sub>

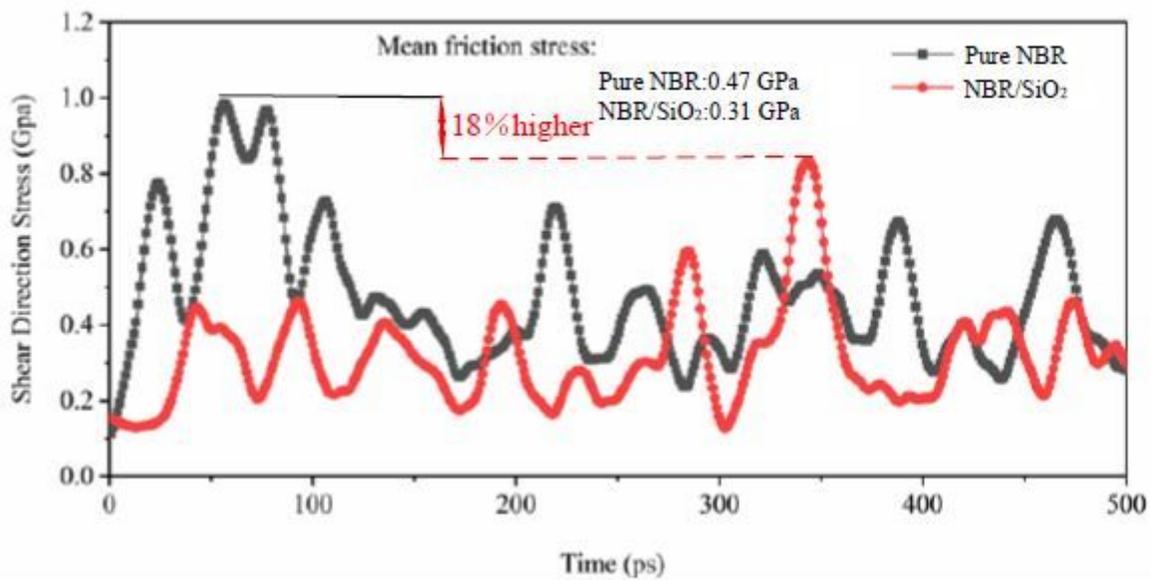


Figure 6

The friction stress between copper atoms and pure NBR (NBR/SiO<sub>2</sub>) during the friction process

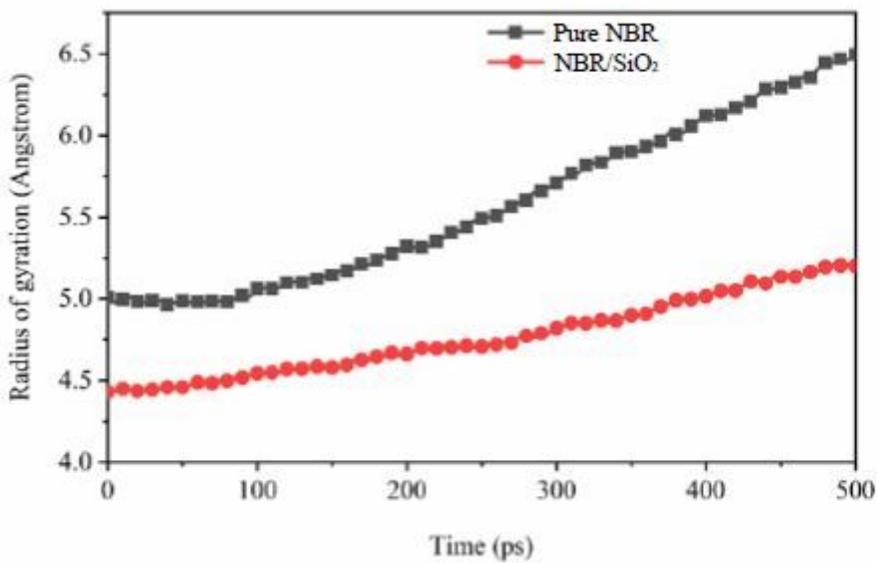
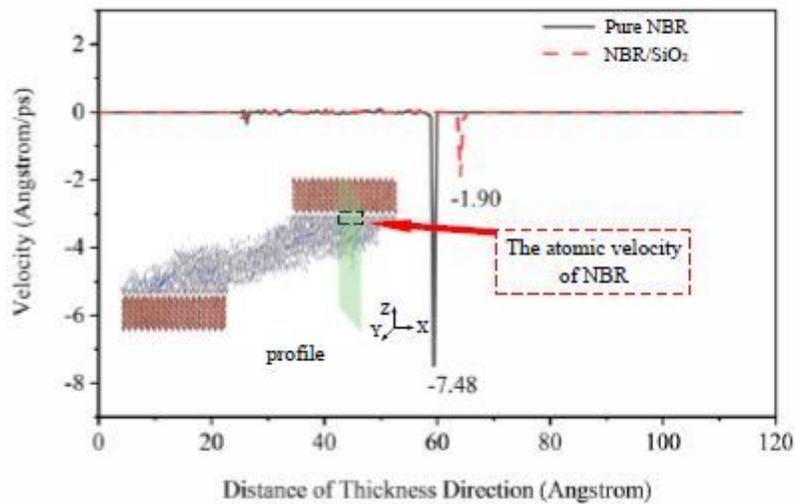


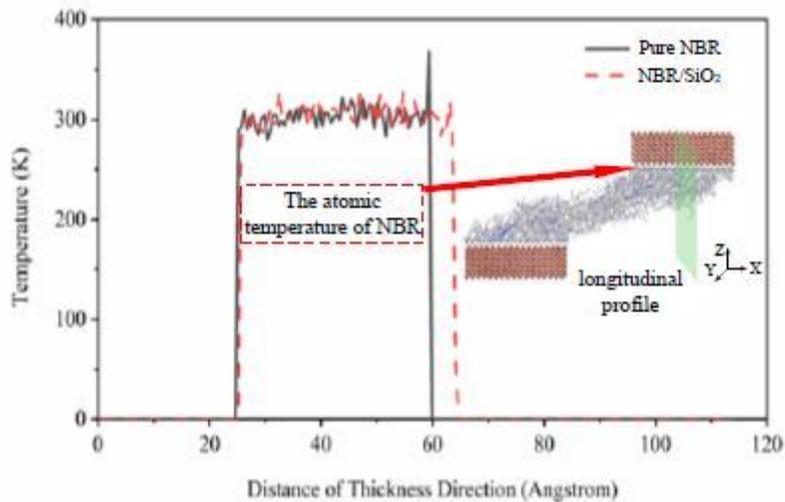
Figure 7

The radius of gyration of NBR molecular chains in pure NBR and NBR/SiO<sub>2</sub> during friction process



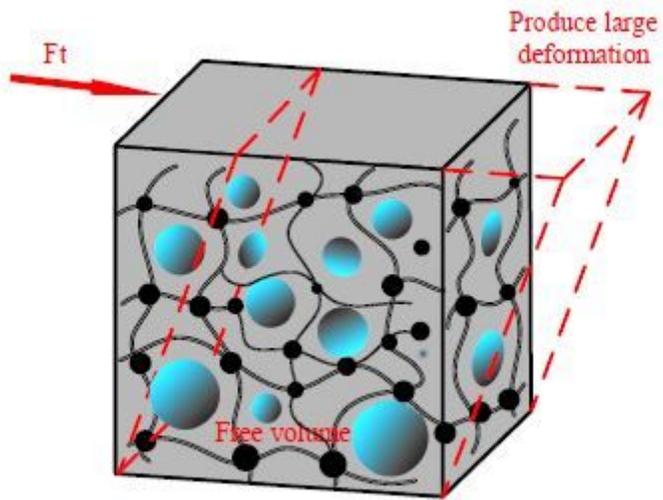
**Figure 8**

Atomic velocity in the longitudinal profile of pure NBR and NBR/SiO<sub>2</sub>

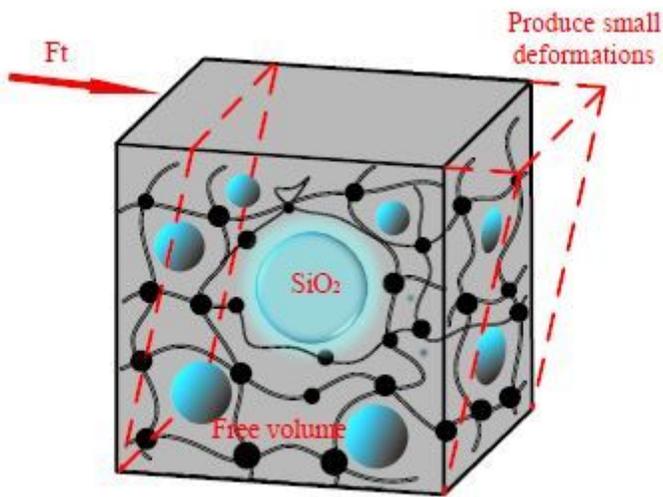


**Figure 9**

Temperature in the longitudinal profile of pure NBR and NBR/SiO<sub>2</sub>



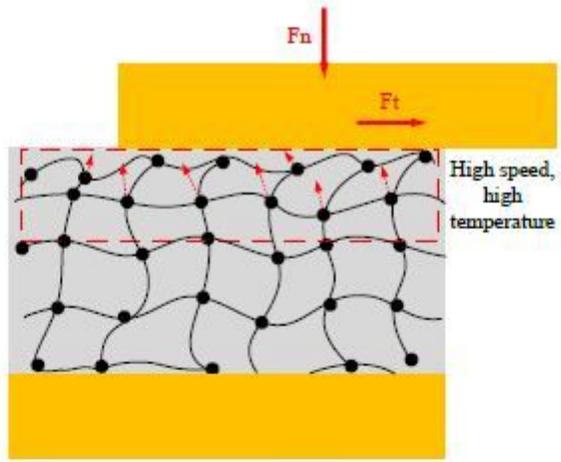
(a)



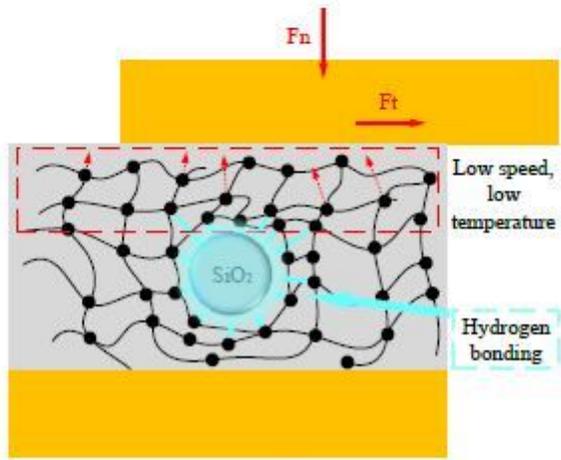
(b)

Figure 10

Schematic of mechanical properties of SiO<sub>2</sub>-reinforced NBR



(a)



(b)

Figure 11

Schematic diagram of tribological properties of SiO<sub>2</sub>-reinforced NBR