

Supplementary Information

Comparative Study of Elastomer Nanocomposites Respectively Containing SWCNTs and MWCNTs

S1. Preparation of CNT thin film for electrical conductivity testing

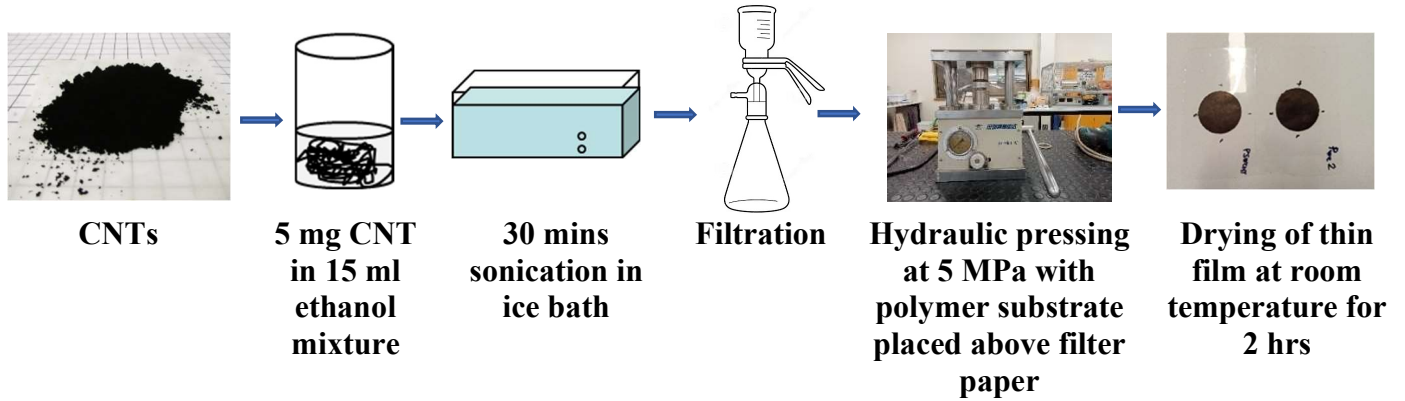


Table S1. Details of thin films for electrical conductivity.

| Nanofiller for the Film | Thickness (cm) | Resistance (Ω) | Electrical Conductivity (S/cm) |
|-------------------------|----------------|-------------------------|--------------------------------|
| SWCNTs | 0.0008 | 0.26 | 1119.16 ± 184 |
| MWCNTs | 0.0018 | 5.97 | 21 ± 2 |

S2. Conversion of Filler Fraction

The fractions of CNTs were changed from weight fraction (W_f) to volume fraction (V_f) using Equation S1 [1];

$$V_f = \frac{\rho_m W_f}{\rho_f (1 - W_f) + \rho_m W_f} \quad (S1)$$

The symbol ρ represents the densities of the involved components whereas subscripts m and f denote the matrix and filler, respectively. The densities of NBR, SWCNTs and MWCNTs are 0.968 g/cm^3 , 1.7 g/cm^3 and 1.8 g/cm^3 , respectively.

References

1. Aakyiir, M., et al., *Combining hydrophilic MXene nanosheets and hydrophobic carbon nanotubes for mechanically resilient and electrically conductive elastomer nanocomposites*. Composites Science and Technology, 2021. **214**: p. 108997. <https://doi.org/10.1016/j.compscitech.2021.108997>.

Standard Operating Procedure for Preparation of Elastomer/CNT Nanocomposites

The information presented comprises a comprehensive set of step-by-step procedures including safety guidelines followed during the preparation of elastomer/carbon nanotube composites.

Experimental framework

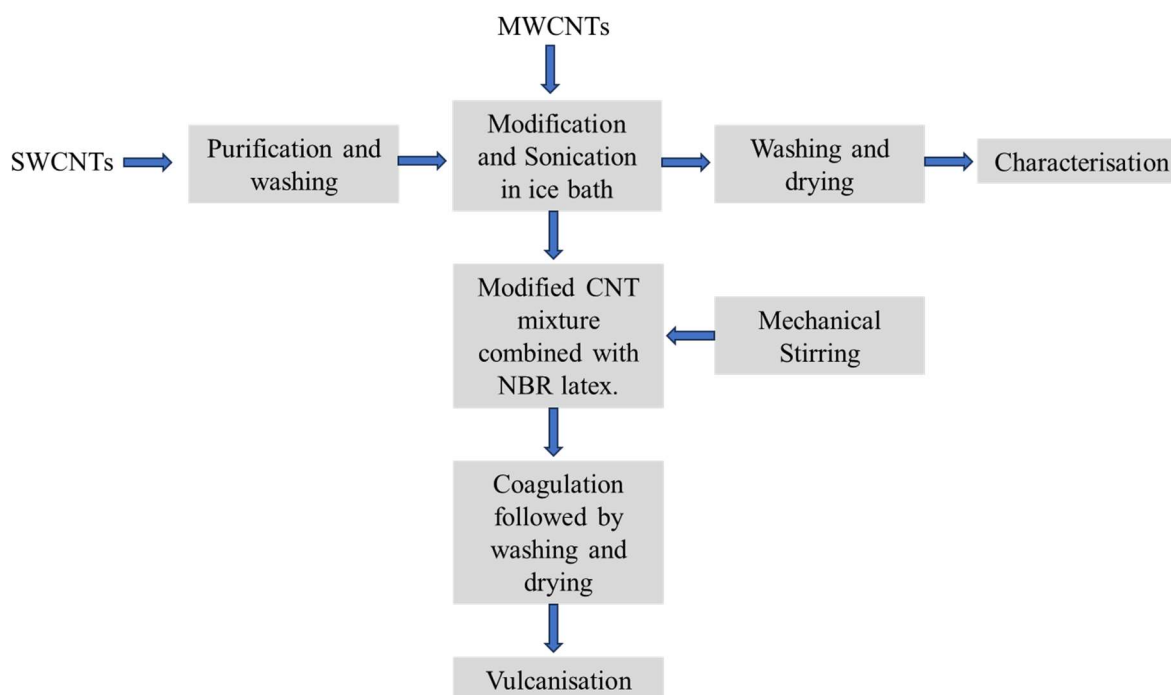


Figure S1. Schematic of elastomer/CNT nanocomposite preparation.

Materials

Purified MWCNTs (model number BT1001M, diameter 10–20 nm and purity > 94%) were obtained from LG Chem Co. Ltd., and SWCNTs were purchased from Techinstro in India. Nitrile butadiene rubber in a latex form (NBR, 630N, 42–43% solid) was procured from NANTEX Industry Co. Ltd in Taiwan. Polyethylene glycol *tert*-octylphenyl ether (Triton X-100) was purchased from Sigma-Aldrich.

Purification of SWCNTs

Identified Hazards

- **Chemical Exposure:** Handling of acids pose a significant chemical exposure risk, including skin and eye irritation, respiratory issues and potential corrosive damage is not managed carefully. It is important to put on the appropriate PPE before handling such chemicals.
- **Refluxing:** The refluxing process involves heating a volatile substance, which can result in the release of toxic fumes. Prolonged exposure to the fumes can be harmful. This process

must be carried out in a fume hood and adequate ventilation must be ensured. Heat gloves must be worn when handling hot fluids.

- **Filtration:** Handling glassware with care is needed at this stage to avoid accidents and injury.

Procedure

To purify the SWCNTs, a reflux process was employed using 250 mg of SWCNTs in a 200 mL solution of nitric acid (HNO_3) with a concentration of 2 M, conducted within a designated chemical fume hood to minimize chemical exposure risk. The purpose of HNO_3 was to remove any amorphous carbon and other carbonaceous impurities. The refluxing procedure was carried out for a duration of 4 hours, with the solution being changed halfway through, specifically after 2 hours. Adequate ventilation was maintained to prevent a build-up of noxious fumes. Once the refluxing was completed, the resulting material underwent filtration while wearing appropriate personal protective equipment (PPE). It was then rinsed with deionised water until reaching a neutral pH.

Subsequently, the material was transferred to a beaker containing 100 ml of 0.2 M HCl solution, with proper chemical handling precautions observed. The mixture was stirred for 30 minutes, and another round of filtration and subsequent washing was carried out. This was done to remove any residual metal catalysts. Finally, the material was dried overnight in a circulator oven at 60 °C, with careful temperature monitoring and safety controls in place. The acid residue obtained after the treatment process was neutralised with sodium hydroxide (NaOH) pellets before discarding.



Figure S2. Reflux setup for the purification of SWCNTs.

Modification of CNTs

Identified Hazards

- **Chemical handling:** TX-100 is a chemical surfactant. While it is not highly hazardous, it is essential to handle it with care and avoid direct skin contact. Appropriate PPEs are required.
- **Filtration:** This involves the handling of glassware. Caution is therefore needed, to avoid accidents and injury.

Procedure

The modification of MWCNTs commenced by dissolving polyethylene glycol tert-octylphenyl ether octylphenol ethoxylate (Triton X-100) in water to form a solution at 1 wt.%. During this step, it is essential to wear appropriate PPEs to prevent any skin contact with TX-100. Subsequently, MWCNTs were added to the solution, and stirring at 250 rpm for 15 minutes was conducted with the apparatus securely fastened to minimize the risk of spills.

To enhance the dispersion of MWCNTs, the resulting mixture was subjected to bath sonication below room temperature for a duration of 45 minutes. Particular attention was paid to cooling measures to prevent the mixture from heating up. After the sonication process, the mixture was washed using deionised water. Subsequently, the material was subjected to a filtration process and then vacuum dried overnight at 60 °C to obtain the modified MWCNTs. It is important to note that a dispersion of CNTs without the drying step was used for latex compounding whereas the dried CNTs were used for characterisation purposes. Throughout this process, safety controls were diligently observed to ensure a safe working environment. The same procedure and standards of safety were applied to the purified SWCNTs to yield modified SWCNTs.

Nanocomposite formulation

Identified Hazard Sections

- **Coagulation:** Handling CaCl_2 solution can pose risks of skin and eye irritation. It is essential to put on the required PPEs.
- **Magnetic stirring:** Ensuring that the apparatus is properly secured is important to avoid the breakage of beakers and potential injury.
- **Vulcanisation Process:** Vulcanisation at 150 °C and 10 MPa involves high temperature and pressure. Safety measures, such as using appropriate PPEs and following proper procedures are crucial to prevent accidents.

Procedure

This study centred on investigating two distinct types of nanocomposites at varying filler fractions (0.56, 1.69, 2.84, 4.02, 5.82 and 7.05 vol.%). Details on the conversion from wt.% to vol.% can be found in section S2 of the supporting information. A suspension of the fillers was carefully added into the NBR latex through magnetic stirring at a controlled speed of 360 rpm for 30 minutes, with the apparatus securely fastened to minimize the risk of spills.

To initiate coagulation, a solution of CaCl_2 was carefully introduced to the mixture at a ratio of 1:1. During this step, handling the CaCl_2 solution with care was paramount to avoid skin or eye irritation, and any accidental splashes were addressed immediately. The resulting coagula were then subjected to thorough washing using deionised water to remove any residual CaCl_2 . Following this, the coagula were meticulously dried overnight within a ventilated oven set at a controlled temperature of 60 °C.

The nanocomposites subsequently underwent further processing through two-roll milling (Figure S3a), incorporating predetermined quantities of vulcanisation agents as specified in Table S1. During this process, 5 rolls and 5 triangles were made. The vulcanisation process was carried out in a curing machine (Figure S3c) under controlled conditions, maintaining a temperature of 150 °C and a pressure of 10 MPa for a duration of 30 minutes. During the vulcanisation process, strict adherence to safety protocols were maintained to ensure a secure working environment. The vulcanisation conditions were predetermined based on the optimised curing curve derived from an oscillating disk rheometer (ZWL-III Rheometer, China) shown in Figure S3b.

Table S2. Vulcanization recipes for nanocomposite.

| Material | Weight (g) |
|--------------------------------------|------------|
| NBR | 100 |
| Sulfur | 1 |
| N, N'-m-phenylenedimaleimide (HVA-2) | 1 |
| Dicumyl peroxide (DCP) | 4 |
| MWCNTs & SWCNTs | Variable |

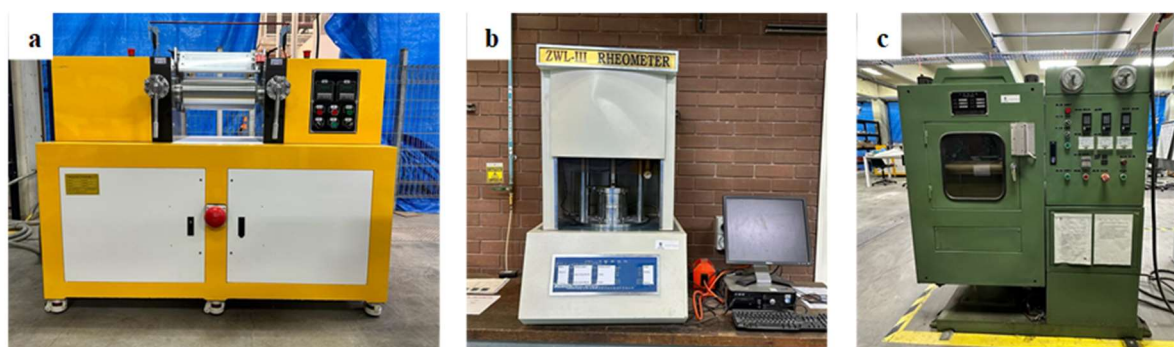


Figure S3. Images of (a) two-roll mill, (b) ZWL-III rheometer and (c) curing machine.