Synthesis, Characterization and Tribological evaluation of TiO₂-Reinforced Boron and Nitrogen Co-doped Reduced Graphene Oxide Based Hybrid Nanomaterials as Efficient Antiwear Lubricant Additives

Vinay Jaiswal[†], Kalyani[†], Sima Umrao[‡], Rashmi B. Rastogi^{†*}, Rajesh Kumar[§] and Anchal Srivastava[‡]

[†]Department of Chemistry, Indian Institute of Technology (Banaras Hindu University) Varanasi-221005, India

[‡]Department of Physics, Banaras Hindu University, Varanasi-221005, India

[§]Department of Mechanical Engineering, Indian Institute of Technology (Banaras Hindu University) Varanasi-221005, India

Corresponding Author: Rashmi Bala Rastogi **Email**: rashmi.apc@iitbhu.ac.in

Fax No. +91 542 2368428

S1. Experimental details

For each experiment arithmetic mean of the diameter of each ball $(d_1,d_2 \text{ and } d_3)$ was taken as given by equation 1. The three stationary balls were not disturbed while taking the readings and the wear scar diameter was taken by tilting eye piece of the microscope at an angle of 35.26^0 making it perpendicular to the surface of the scar.

S1.1. Tribological Parameters

S1.1.1. Mean wear scar diameter (MWD)

$$d = \frac{d_1 + d_2 + d_3}{3}$$
 1

S1.1.2. Mean wear volume (MWV)

Wear volume,
$$V = \frac{\prod d_0^4}{64 r} \{ (\frac{d}{d_0})^4 - (\frac{d}{d_0}) \}$$
 2

Hertzian diameter,
$$d_0 = 2(\frac{3Pr}{4E})^{\frac{1}{3}}$$
 3

Where, $\frac{1}{r} = \frac{1}{r_1} + \frac{1}{r_2}$

$$\frac{1}{E^*} = \frac{1 - v_1^2}{E_1} + \frac{1 - v_2^2}{E_2}$$

Where, E^* = Resultant modulus of elasticity

v = Poissons ratio

r = Radius of steel ball

$$E_1 = E_2 = 206 \text{ GPa}$$

$$v_1 = v_2 = 0.3$$

P = Actual load in Newton on each of the three horizontal balls that is 0.408 times of applied load.

S1.1.3. Wear rate

Overall, running-in and steady-state wear rate have been calculated on the basis of observed mean wear volume data at different time intervals. Mean wear volumes at different times (15, 30, 45, 60, 75 and 90 min.) for each experiment were plotted with time and a linear regression model was fitted on the points including origin to find out overall wear rate.

$$\frac{V}{l} = K \frac{P}{H}$$

V = mean wear volume

- l = sliding distance (2 π r.N)
- K = wear coefficient
- H = hardness of steel ball (59-61 HRC)
- P = applied load (0.408x392N)



Figure S1. Raman spectra of studied MRGs sample



Figure S2. Raman spectrum of TiO₂ nanoparticle



Figure S3. XPS survey of MRG and TiO₂-B-N-MRG samples



Figure S4. Dispersion stabilities of the pure oil containing MRG, B-N-MRG and TiO_2 -B-N-MRG studied by UV-vis spectrophotometry (a), Optical photographs of the different MRGs samples dispersed in pure oil at different settling times (b)



Figure S5. Variation of mean wear scar diameter with time for paraffin oil containing 0.15% w/v of different MRGs nanomaterials at 392N applied load



Figure S6. Variation of mean wear volume with time for paraffin oil containing 0.15% w/v of different MRGs nanomaterials at 392N applied load



Figure S7. Determination of running-in wear rate by varying mean wear volume with time (h) for paraffin oil containing (0.15% w/v) MRGs based nanomaterials at 392N applied load



Figure S8. Determination of steady-state wear rate by varying mean wear volume with time (h) for paraffin oil containing (0.15% w/v) MRGs based nanomaterials at 392N applied load



Figure S9. SEM micrographs at different magnifications of the worn steel surface lubricated with different additives (0.15% w/v) in paraffin oil for 30 min test duration at 588 N applied load: (a) MRG, (b) B-MRG, (c) B-N-MRG and (d) TiO₂-B-N-MRG



Figure S10. 2*D* and 3*D*-AFM images of the worn steel surface lubricated with different additives (0.15% w/v) in paraffin oil for 30 min test duration at 588 N applied load: (a) MRG, (b) B-MRG, (c) N-MRG, (d) B-N-MRG and (e) TiO₂-B-N-MRG