SUPPORTING INFORMATION

Hybrid MoS_2/h-BN Nanofillers As Synergic Heat Dissipation and Reinforcement Additives in Epoxy Nanocomposites

Hélio Ribeiro[1,2*], João Paulo C. Trigueiro[2,3], Wellington M. Silva[2], Cristiano F. Woellner[1,4], Peter S. Owuor[1], Alin Cristian Chipara[1], Magnovaldo C. Lopes[2], Chandra S. Tiwary[1], Jairo J. Pedrotti[1,5], Rodrigo Villegas Salvatierra[6], James M. Tour[6], Nitin Chopra[7], Ihab N. Odeh[7], Glaura G. Silva[2], Pulickel M. Ajayan[1].

*Corresponding author: helioribeiro@hotmail.com

1- Department of Materials Science and Nanoengineering - Rice University. 6100 Main St, Houston, TX, 77005 USA.
2- Departamento de Química - Universidade Federal de Minas Gerais. Av. Antônio Carlos, 6627 – Pampulha, CEP 31270-901, Belo Horizonte - MG, Brazil.
3- Instituto Federal de Minas Gerais - Campus Congonhas. Av. Michael Pereira de Souza, 3007 - Campinho, CEP 36415-000, Congonhas - MG, Brazil.
4- Departamento de Física Aplicada - Universidade Estadual de Campinas. Rua Sérgio Buarque de Holanda, 777 - CEP 13083-859, Campinas, SP, Brazil.
5- Centro de Pesquisas Avançadas em Grafeno, Nanomateriais e Nanotecnologias - Universidade Presbiteriana Mackenzie. Rua da Consolação, 930, CEP 01302-907, São Paulo - SP, Brazil.
6- Department of Chemistry Rice University- 6100 Main St, Houston, TX, 77005 USA.
7- SABIC Americas Inc, Sugar Land, TX 77478, USA.

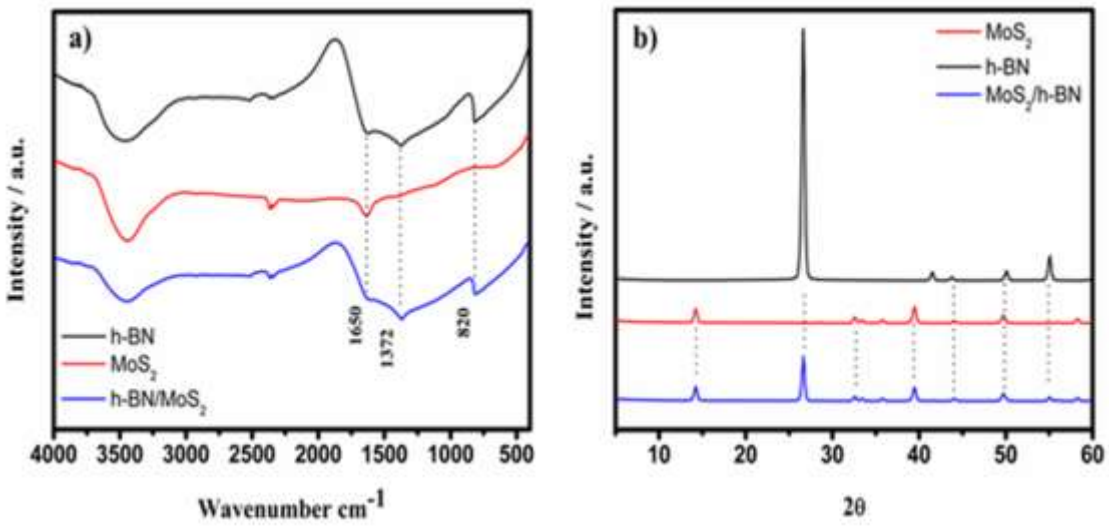

Figure S1. (a) FTIR spectra and (b) XRD patterns of MoS_2, h-BN and hybrid MoS_2/h-BN material. The dash lines indicate the correspondence in the signals for the hybrid composite and the pure nanomaterials.

The FTIR spectra of h-BN, MoS_2, and mixture of h-BN/MoS_2 (Figure S1a), show the main characteristic peaks, which are considered fingerprints of sp^2 bonds of h-BN: at 1372 cm^{-1} corresponding to the in-plane B–N transverse stretching and 820 cm^{-1} corresponding to the out-of-plane B–N–B bending vibration.[1] The broad band around ~3428 cm^{-1} can be attributed by the residual bonded N-H or caused to the water molecules absorbed on the surface of the samples.[1-4] The vibrational modes at ~3435 and 1650 cm^{-1} are assigned to hydroxyl functionalities of adsorbed moisture on the MoS_2 nanosheets.[5]

The XRD patterns of h-BN, MoS_2, and mixture of h-BN/MoS_2 are shown in Figure S1b. The intense diffraction peak 2θ ~26.76°, (002) plane, denote the high crystallinity of the h-BN nanostructure.[1] MoS_2 showed characteristic peaks at 2θ of 12.00°, 32.00°, 40.00°, and 50.01° due to diffraction from (002), (100), (103), and (105) planes, respectively.[5]

The diffraction pattern was found to be fully matched with JCPDS file 37-1492. The sample of the heterostructure h-BN/MoS_2 showed peaks corresponding to both h-BN and MoS_2 separated samples.

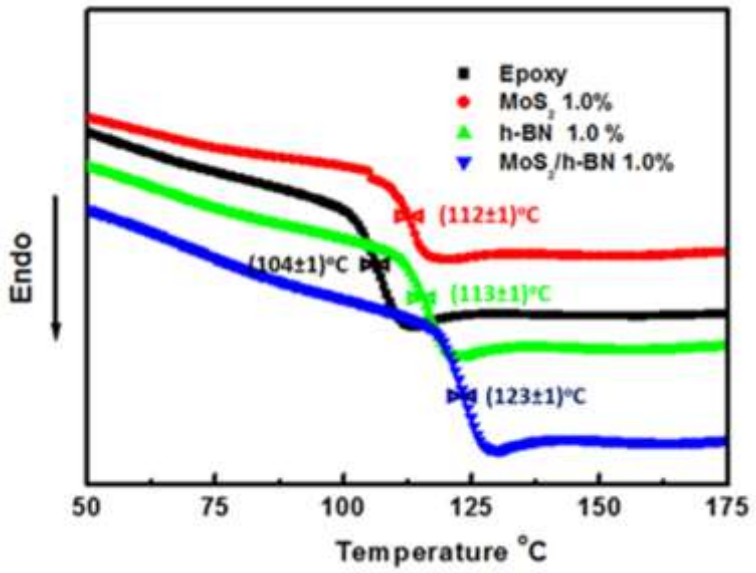

Figure S2. DSC curves of neat epoxy and composites containing 1.0 wt.% of MoS_2, h-BN and hybrid MoS_2/h-BN.

DSC curves for pure epoxy and the composites containing 1.0 wt% of MoS_2, h-BN and MoS_2/h-BN in the second heating scan are shown in Figure S2. The glass transition temperature (T_g) was determined from the midpoints of three measurements (average values) for each sample. The T_g values showed standard deviation of ± 1°C. Increases in T_g values for all systems were observed, however, the system containing 1.0 wt % of MoS_2/h-BN showed the best increase of up to 19ºC when compared to pure polymer. Generally, in epoxy systems the increase of the glass transition temperature is associated with restriction of the mobility of their polymer chains due to a high degree of cross-link and reduction of free volume.[6] Factors that affect the value of T_g for epoxy nanocomposites include: the degree of dispersion of the nanofillers, interaction between

nanofillers/polymer and curing process conditions. Under the conditions studied here, it can be said that the cross-linking process was not affected by the addition of nanofillers, i.e., the polymer chains were not generated with free ends as observed by other authors.[7] Moreover, it is possible that the interface between the introduced MoS_2 and h-BN served as chemical anchor points for epoxy chains, thus impacting the mobility thereof and increasing the T_g values in the hydride composite.

Table S1. Storage modulus, T_g and cross-link density values of neat epoxy and nanocomposites with different wt% of 2D nanofiller

System (wt%)	Storage Modulus at T_g (MPa)	T_g (ºC) ±1	Cross-link Density (mol cm^{-3})
Neat epoxy	1662±13	123	0.5056±0,0011
MoS_2 0.25	1642±11	125	0.5289±0,0015
MoS_2 0.50	1725±21	126	0.5312±0,0008
MoS_2 1.0	1738±19	126	0.5828±0.0014
h-BN 0.25	1613±22	127	0.5013±0.0013
h-BN 0.50	1645±27	128	0.5343±0.0010
h-BN 1.0	1637±29	130	0.6371±0.0011
MoS_2/ h-BN 0.25	2627±22	131	0.5917±0.0014
MoS_2/ h-BN 0.50	2674±26	133	0.6273±0.0012
MoS_2/ h-BN 1.0	2777±18	135	0.7183±0.0013

The values of brittleness (B) for viscoelastic materials enables the comparative analysis of several types of polymer-based materials, metal, alloys, ceramics and glasses.[8] The parameters obtained from tensile testing can be connected with the brittleness through the equation proposed by Brostow and Narkis. [9]

$$B = {}^{1}/_{(\varepsilon_b\, E')} \quad (2)$$

where ε_b is the tensile elongation at break, and E' is the storage modulus determined by DMA test at 1 Hz, both at same temperature. [8-10]. The numerical values of storage modulus, tensile elongation and brittleness at 25ºC for neat epoxy and nanocomposites are shown in Table S2.

Table S2. Storage modulus (E'), tensile elongation at break (ε_b), and brittleness (B) values of neat epoxy and nanocomposites with different wt% of 2D nanofiller at 25ºC

System (wt%)	E' (Pa)/10^8	ε_b (%)	B (%Pa/10^{10})
Neat epoxy	44.49± 09	15.28	0.147
MoS_2 0.25	46.72± 11	18.69	0.115
MoS_2 0.50	46.35±13	20.27	0.106
MoS_2 1.0	44.25±15	19.38	0.116
h-BN 0.25	48.28±07	19.83	0.104
h-BN 0.50	49.54±17	19.85	0.102
h-BN 1.0	50.21±14	17.56	0.113
MoS_2/ h-BN 0.25	56.68± 10	18.33	0.093
MoS_2/ h-BN 0.50	55.24±15	21.76	0.081
MoS_2/ h-BN 1.0	59.97±12	23.25	0.074

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