Supporting Information

Dopamine@Nanodiamond as Novel Reinforcing Nanofillers for Polyimide with Enhanced Thermal, Mechanical and Wear Resistance Performance

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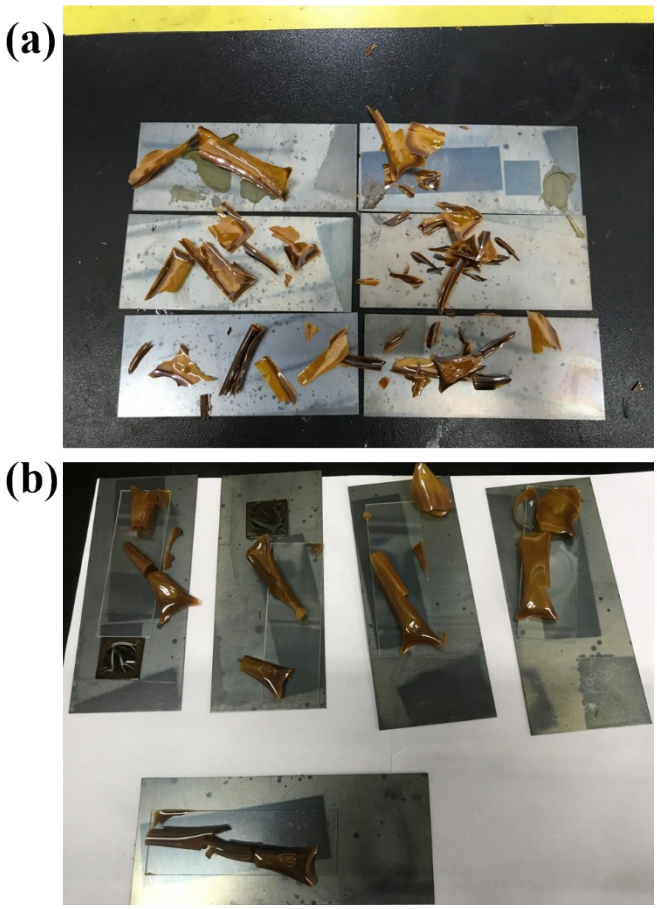

Fig.S1. Photograph of PI/PDA-ND Composites (a) 1.5 wt % PI/PDA-ND (b) 2 wt % PI/PDA-ND

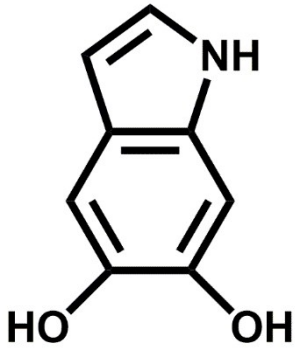

Fig.S2. the structure of polydopamine structural unit

As shown in Fig.S2, we choose a simple and calculable model of polydopamine molecule, and the plane-wave energy cutoff of polydopamine structural unit was set at

650 eV, the K point was set at 1×1×1. On the other hand, the plane-wave energy cutoff of diamond was set at 450 eV, and the K point was set at 1×1×1. The typical computational formula is $E = E_{12}-(E_1+E_2)$, and the results are as follow:

For the interaction between ND and PDA:

$E_{system}=E_{12}=-8.59017784\times10^3$

$E_{diamond}=E_1=-6181.78743$

$E_{polydopamine}=E_2=-2.40219749\times10^3$

$E=-8.59017784\times10^3-(-6181.78743-2.40219749\times10^3)$

$=-8590.17784+8583.98492$

$=-6.19292$ eV

For the van der Waals forces of ND：

$E_{system}=E_{12}=-1.23850548\times10^4$

$E_{diamond}=E_1= E_2=-6181.78743$

$E'=-1.23850548\times10^4-(-6181.78743\times2)$

$=-12385.0548+12363.57486$

$=-21.47994$ eV

Based on the results, we found that the interaction between ND and PDA is slightly smaller than the van der Waals forces of ND. But the structure of polydopamine which used to calculate is too simple, it is difficult for us that calculate the interaction between ND and PDA using complicated polydopamine structure. And the most researches using polydopamine structure to calculate was complex. For example, Deng et al used PDA tetramer as model to calculate the interaction between the PDA and the lithium sulfides. (Deng et al Durable Polydopamine-Coated Porous Sulfur Core–Shell Cathode for High Performance Lithium–Sulfur Batteries. *Journal of Power Sources* **2015,** *300*, 386-394) On the other hand, the XPS and XRD of nanodiamond indicated that ND contains a certain amount of graphite structure, due to the uncertainty of the graphite content, and the large, complex calculation, the force of this part is not added to the interaction between ND and PDA, the actual interaction force would be greater than the result of the above calculation.

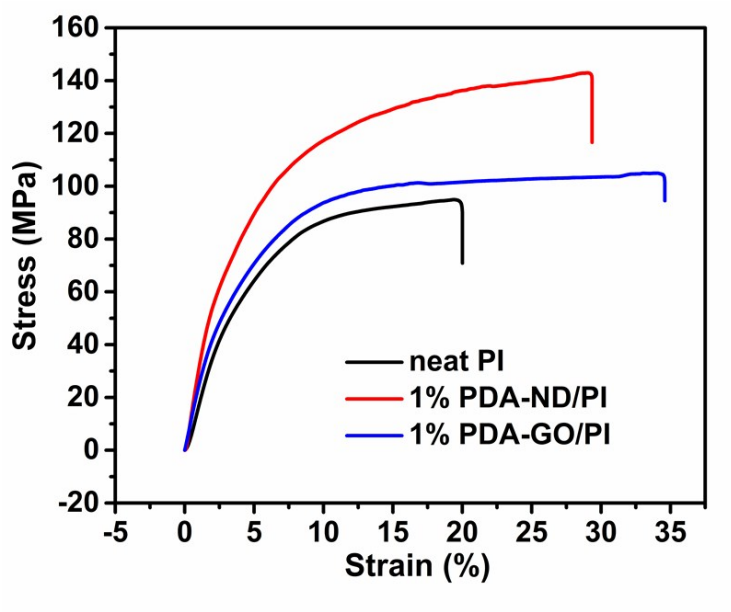

Fig.S3. Tensile performances of neat polyimide, 1 wt % PI/PDA-GO composites and 1 wt % PI/PDA-ND composites.

As shown in Fig.S3, we compared the tensile property of 1 wt % PDA-GO/PI and 1 wt % PDA-ND/PI. It is obvious that the tensile strength of 1 wt % PDA-ND/PI composites (138 MPa) higher than 1 wt % PDA-GO/PI composites (106 MPa).

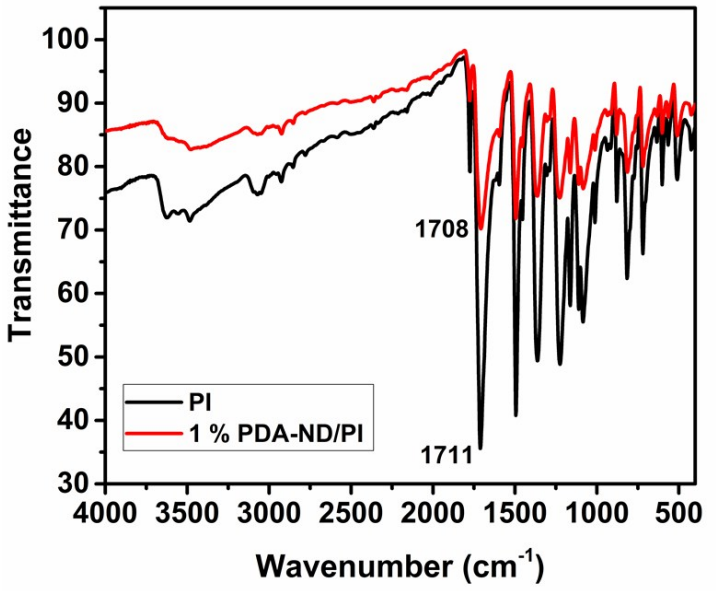

Fig .S4. FTIR of pure PI and 1 wt % PDA-ND/PI nanocomposite

As shown in Fig. S4，the absorption peaks of PI at 1711 cm^{-1} due to C=O stretching vibration, while the 1 wt % PDA-ND/PI nanocomposite showed wider

absorption peaks at the same position compared with pure PI. It is indicated that C=O bond weaken due to the hydrogen bonding between polyimide and polydopamine.

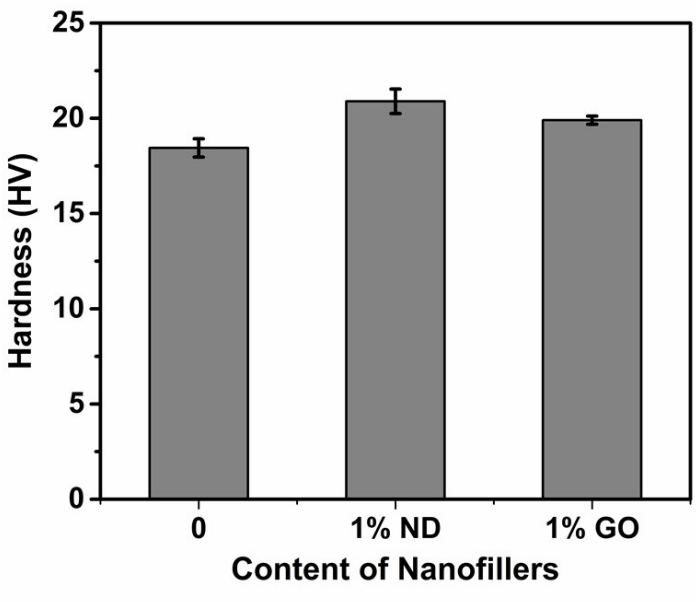

Fig.S5. Vickers hardness of neat polyimide, 1 wt % PI/PDA-ND composites and 1 wt % PI/PDA-GO composites.