Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supporting Information

Bonding-induced thermal transport enhancement across hard/soft materials interface using molecular monolayers

Chao Yuan, Mengyu Huang, Yanhua Cheng and Xiaobing Luo*

State Key Laboratory of Coal Combustion, School of Energy and Power Engineering,

Huazhong University of Science and Technology, Wuhan 430074, China.

*E-mail: luoxb@hust.edu.cn

Supplementary Figures

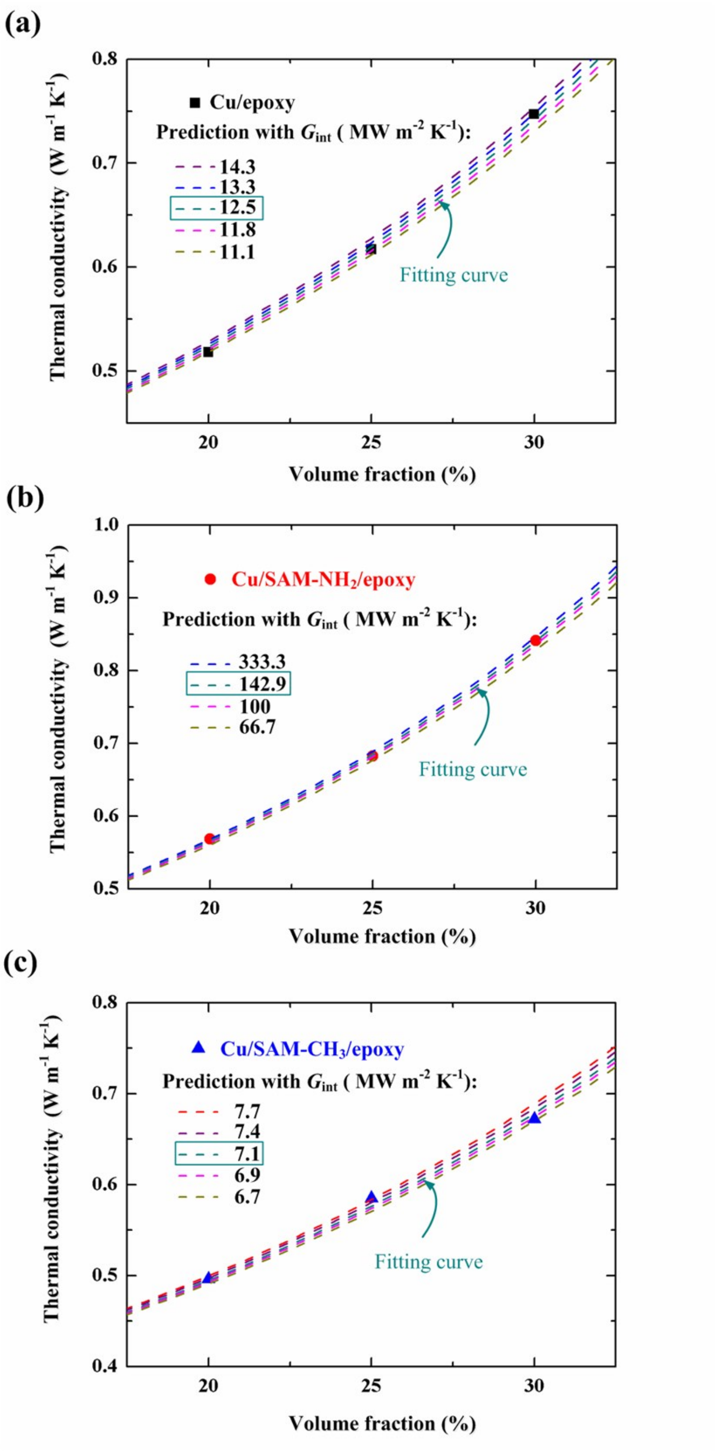

Figure S1. Data fitting to extract G_{int} of (**a**) Cu/epoxy, (**b**) Cu/SAM-NH_2/epoxy and (**c**) Cu/SAM-CH_3/epoxy interfaces. Dots: measured thermal conductivity of composites; Colored dash lines: predicted thermal conductivity from EMBM with different values of G_{int}.

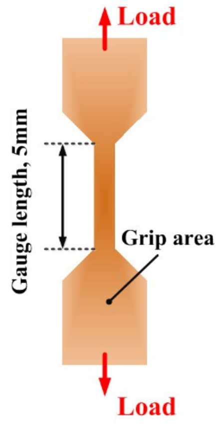

Figure S2. Schematic of the tensile test.

Supplementary Tables

Table S1. Data of density, heat capacity, thermal diffusivity and thermal conductivity of copper and epoxy resin.

Materials	Density ρ (g cm^{-3})	Heat capacity C_p (J g^{-1} K^{-1})	Thermal diffusivity α (mm^2 s^{-1})	Thermal conductivity k (W m^{-1} K^{-1})
Copper	8.9 [1]	0.388[1]		401[1]
Epoxy resin	1.1 [2]	1.669[a]	0.159[b]	0.292[c]

[a] measured by a differential scanning calorimetry (Diamond DSC, PerkinElmer Instruments); [b] measured by LFA467; [c] calculated according to the formula: $k=\alpha C_p\rho$.

Tables S2. Data of effective density, heat capacity, thermal diffusivity and thermal conductivity for the composites at volume fraction of 20%, 25% and 30%.

f (%)	ρ (g cm^{-3})	w (%)	C_p (J g^{-1} K^{-1})	α (mm^2 s^{-1})	k (W m^{-1} K^{-1})

				Cu/epoxy	Cu/ SAM-NH_2/ epoxy	Cu/SAM-CH_3/ epoxy	Cu/ epoxy	Cu/ SAM-NH_2/ epoxy	Cu/ SAM-CH_3/ epoxy
20	2.692	66.12	0.822	0.237	0.26	0.227	0.5182	0.8410	0.672
25	3.080	72.24	0.744	0.272	0.301	0.258	0.6169	0.6827	0.5851
30	3.468	76.98	0.683	0.318	0.358	0.284	0.7470	0.5685	0.4963

Supplementary Notes

1. Cu modification with SAMs

Dodecanethiol (SAM-CH_3):

1mM ethanolic solution was prepared by dissolving 0.0072 mL of dodecanethiol into 30 mL of ethanol. Subsequently, 5g of Cu powders were immersed into the solution and magnetically stirred for 24h at 25°C. The treated samples were then removed from the solution and rinsed thoroughly with ethanol before air drying.

11-Amino-1-undecanethiol hydrochloride (SAM-NH_2):

1mM ethanolic solution was prepared by dissolving 0.0072g of 11-Amino-1-undecanethiol hydrochloride into 30 mL of ethanol. Subsequently, 5g of Cu powders were immersed into the solution and magnetically stirred for 24h at 25°C. The treated samples were then removed from the solution and rinsed thoroughly with ethanol before air drying.

2. Calculation of effective C_p and ρ

$$C_{\mathrm{p}} = wC_{\mathrm{cop}} + (1-w)C_{\mathrm{epoxy}} \tag{S1}$$

where w is the weight percentage of copper powders in composites. C_{cop} and C_{epoxy} are the heat capacity of copper and epoxy, respectively, which are provided in Table S1.

$$\rho = f\rho_{\mathrm{cop}} + (1-f)\rho_{\mathrm{epoxy}} \tag{S2}$$

where f is the volume faction of copper powders in composites. ρ_{cop} and ρ_{epoxy} are the density of copper and epoxy, respectively, which are provided in Table S1. The calculated results are summarized in Table S2.

3. Extraction of G_{int} for Cu/epoxy, Cu/SAM-NH_2/epoxy and Cu/SAM-CH_3/epoxy interface

Firstly, we used MBAM to predict k_{eff} under a variety of G_{int} values. A portion of the predicting results are provided in Fig. S1. Now, G_{int} can be extracted by fitting the measured thermal conductivity to one of the predicting curves. In order to obtain the precise fitting results, a variable, s, is introduced:

$$s = \sum_{f} (k_{\mathrm{p}\text{-}f} - k_{\mathrm{m}\text{-}f})^2 \qquad f\text{=20\%, 25\%, 30\%} \tag{S3}$$

where $k_{\mathrm{p}\text{-}f}$ and $k_{\mathrm{m}\text{-}f}$ are the predicted and measured thermal conductivity of composites at the volume fraction of f. The G_{int} under which $k_{\mathrm{p}\text{-}f}$ makes s minimal is the optimal fitting result. Figure S1 gives the fitting results for the Cu/epoxy, Cu/SAM-NH_2/epoxy and Cu/SAM-CH_3/epoxy systems, respectively.

References

1. C. P. Dillon, *CRC Materials Science and Engineering Handbook*, Third edition, Access Intelligence, LLC, 2002.
2. Huntsman International LLC. Data sheet of epoxy resin. Available from: http://www.huntsman.com/advanced_materials/a/Your%20Industry/Coatings?p_langswitch=1. Accessed: 2016-07-5.