Reduction of Interfacial Thermal Resistance of Overlapped Graphene by Bonding Carbon Chains

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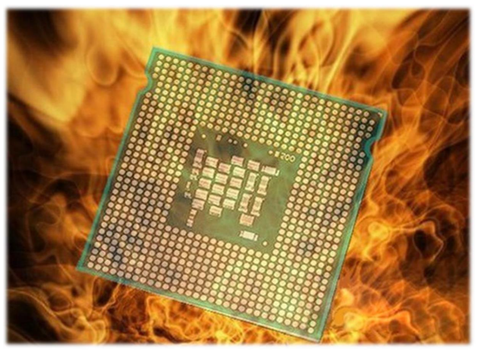
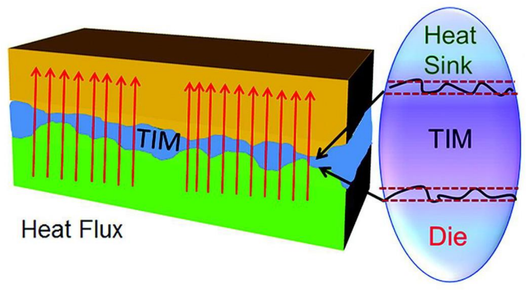
Background





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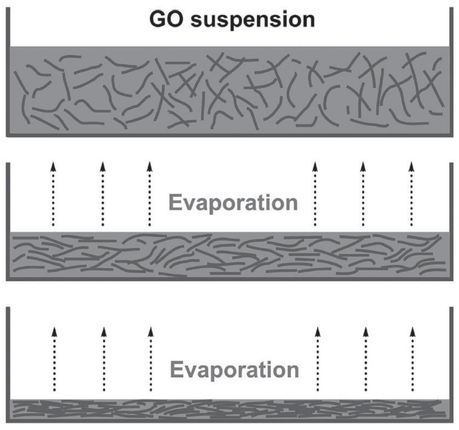

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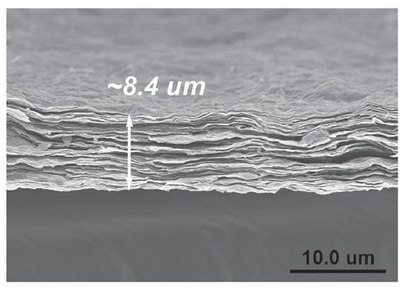

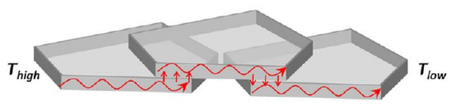

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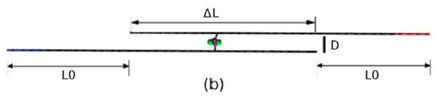

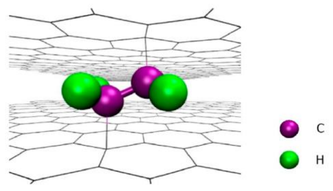

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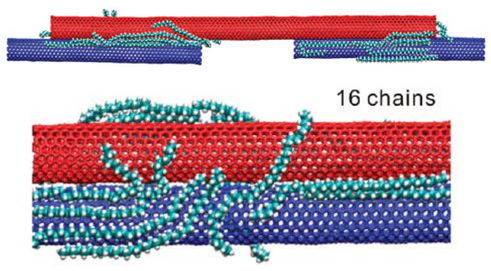
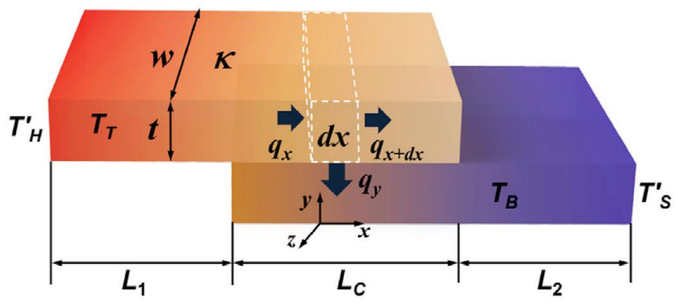


ACS nano 3, 2767-2775 (2009)

Cross-interface Model (CIM)



Mater. Today Phys., 100139 (2019)

$$R_{intra} = \frac{R}{2} = \frac{L_C}{2\kappa A}$$

$$R_{inter} = \frac{1}{G_{CA} w L_C}$$

$$\gamma = \sqrt{2\, G_{CA} w / \kappa A}$$

Temperature distribution functions:

$$T_T = \frac{1}{2}(a \times e^{-\gamma x} + b \times e^{\gamma x} + cx + d)$$

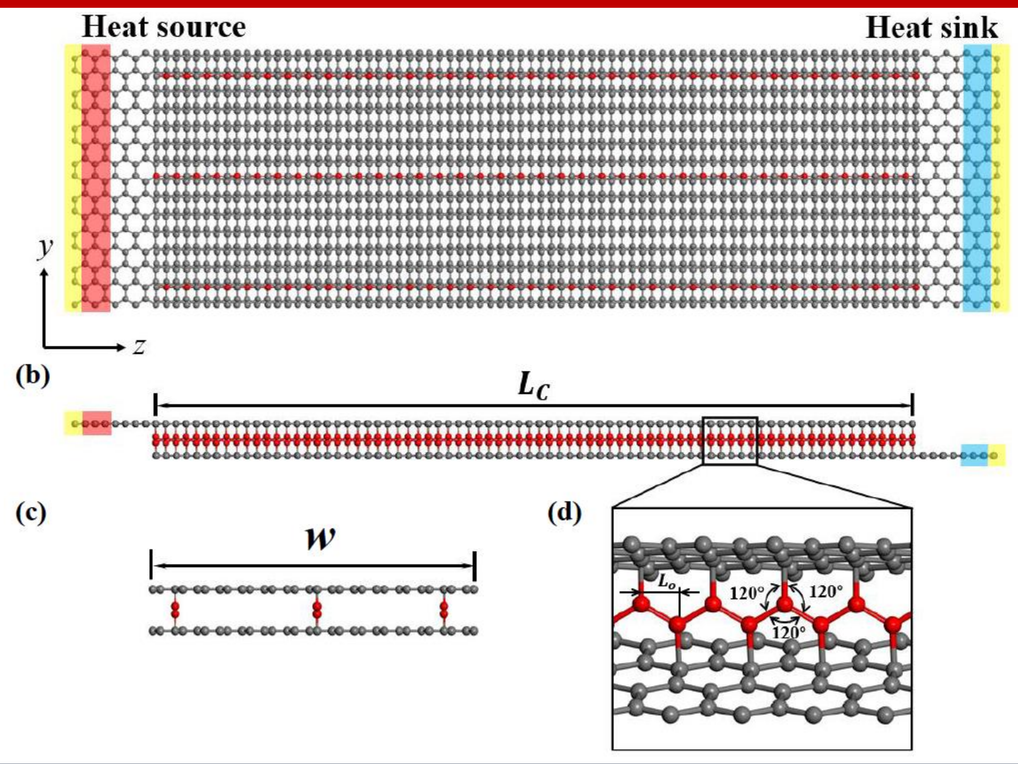
$$T_B = \frac{1}{2}(-a \times e^{-\gamma x} - b \times e^{\gamma x} + cx + d)$$

Thermal resistance:

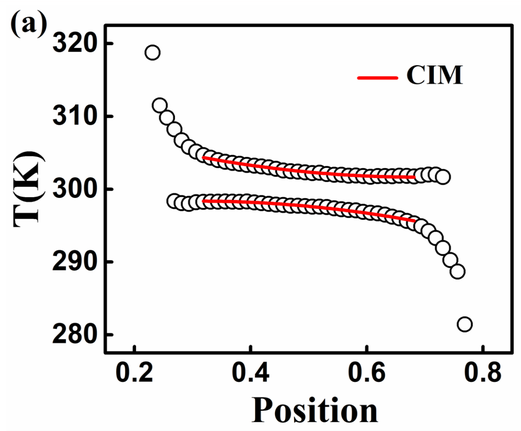
$$R_{total} = R_{intra} + \frac{1}{\eta} \times R_{inter} \qquad \eta = \frac{tanh\sqrt{R_{intra}/R_{inter}}}{\sqrt{R_{intra}/R_{inter}}}$$

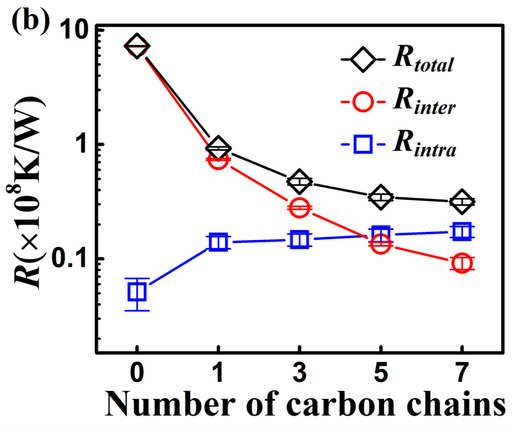
Phys. Chem. Chem. Phys. 21, 25072-25079 (2019)

NEMD Model

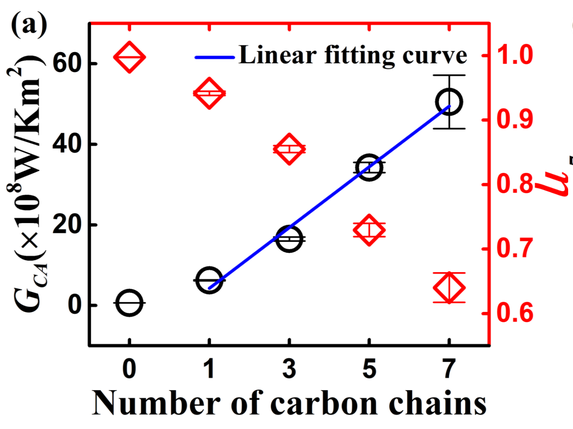


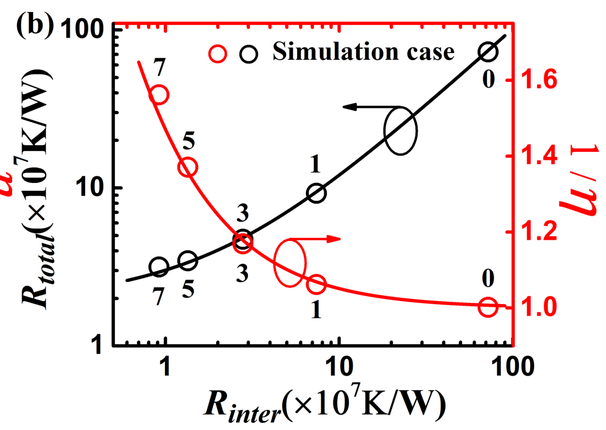
Results and Discussion



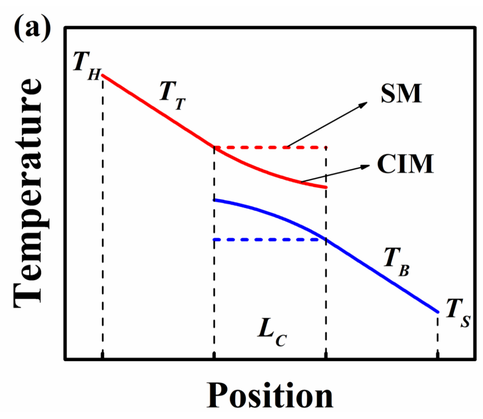


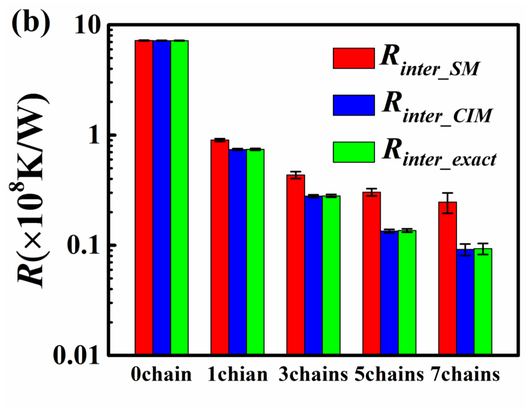
With one carbon chain, The R_{total} and R_{inter} can be reduced by almost one order of magnitude, from $7.27 \times 10^8\ K/W$ and $7.20 \times 10^8\ K/W$ to $9.25 \times 10^7\ K/W$ and $7.40 \times 10^7\ K/W$, respectively.





The interfacial thermal conductance per unit area nearly follows a linear relationship with the number of carbon chains. And a roughly proportional relationship ($R_{inter} \propto 1/\sqrt{N}$) can be deduced.





CIM can exhibit two-dimensional thermal transport process and obtain clear temperature distribution profile which make it possible to directly calculate R_{inter_CIM} accurately.

Summary

- After one carbon chain is bonded, the interfacial thermal resistance is reduced by an order of magnitude.
- While more carbon chains are bonded, the decreasing rate of interfacial thermal resistance slows down gradually.
- The advantage of CIM relative to the traditional simplified model is demonstrated in the example of overlapped GNRs especially when more carbon chains are bonded.
- Our study can provide valuable guide for the design and application of graphene-based materials for effective thermal management and modulation.

Acknowledgments

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