Dynamic Thermal Interface Material (D-TIM) Simulation and Parameter Optimization Using Genetic Algorithm

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Anchor Science LLC, led by Dr. Ewa Kirkor, invented D-TIM, which is a nanocomposite mixture of multi-wall carbon nanotubes and nano-graphites [1] shown in figure 1 (a). D-TIM is an adaptive thermal interface material that dynamically adapts its thermal conductivity with temperature and, as a result, the thermal conductivity of D-TIM increases as temperature increases unlike that of the state-of-the-art TIMs: this quality makes D-TIM a promising thermal interface material with faster and more efficient heat delivery.

To study the nature of D-TIM, we implemented a percolation theory-based simulation which incorporates resistive circuit network model [2]. The model takes into account the geometry of D-TIM sitting between CPU chip surface and heatsink. In addition, thermo-electric effect and variable range hopping conductance were employed to capture its thermal conductivity trend. Our simulation framework creates random D-TIM geometry based on mass ratio of D-TIM elements, simulates the temperature and potential change by updating the electric current and heat flux. Finally, it outputs the effective thermal conductivity of the system.

With the percolation theory-based simulation being our core physical engine, we use genetic algorithm to deduce the optimal parameter values that provide best fitness to the measurement data. This optimization algorithm makes us able to perform data-driven simulation by estimating the values of 45 parameters that include the thermal conductivity and electric conductivity for all elements and their contact properties. Simulation results with the optimized parameters show good agreement with the linear fit of the measurement data as in figure 5.

In this work, we present percolation theory-based simulation framework that captures and predict the effective thermal conductivity trend of D-TIM and the optimization procedure to reverse engineer the physical parameters for data-driven simulation.

[1] E. S. Kirkor, A. D. Schricker, S. K. Sinha, and A. Scheeline, U.S. Patent US 2014/0345843 A1 (2014)
[2] M. Jo, Ph.D. dissertation, University of Illinois at Urbana-Champaign (2018)

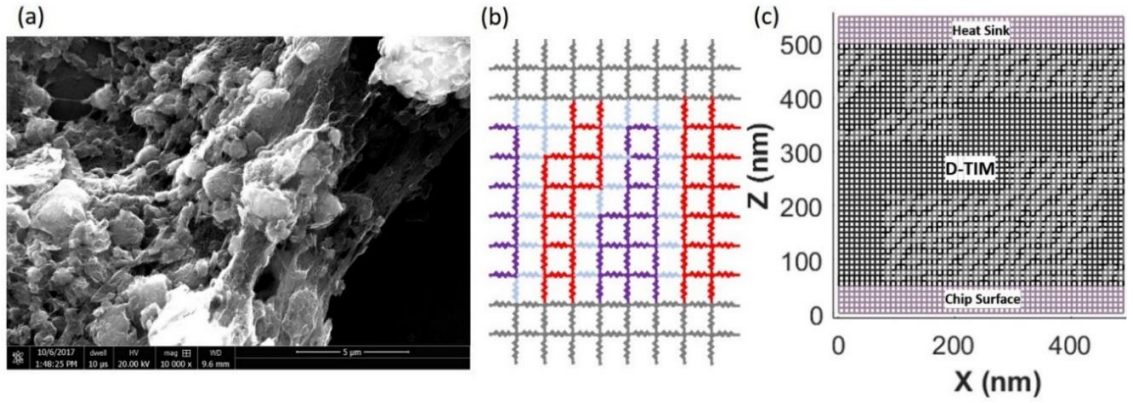

Fig.1: (a) Environmental Scanning Electron Microscope (ESEM) image of D-TIM sample. MWCNTs are tangled and covering the nGs. (b) Resistive network example for D-TIM percolation simulation. (c) Example of D-TIM percolation simulation setup.

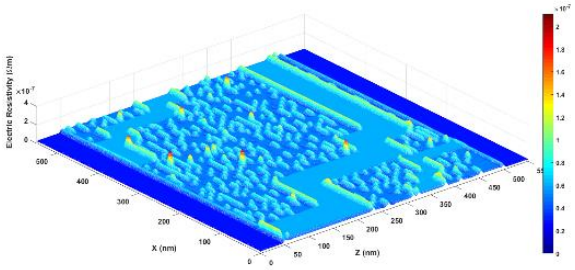

Fig.2: Electric resistivity ρ assigned to branches of D-TIM simulation. ρ_z, the vertical branches in the Z-direction.

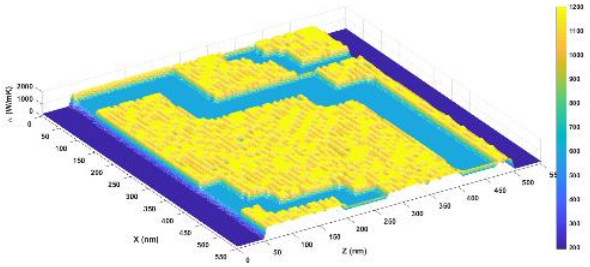

Fig.3 Thermal conductivity κ_z assigned to branches of D-TIM simulation.

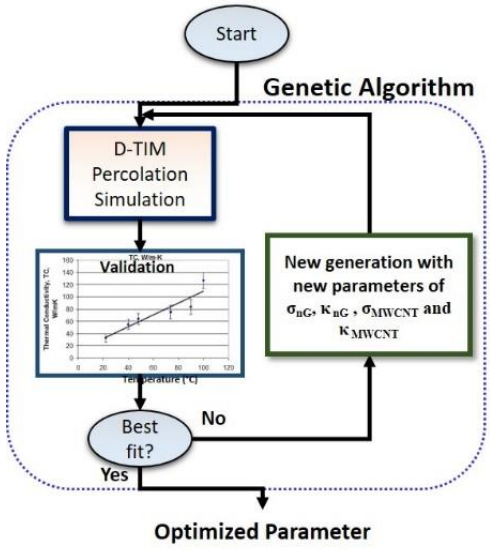

Fig.4: The pipeline for D-TIM parameter optimization using genetic algorithm.

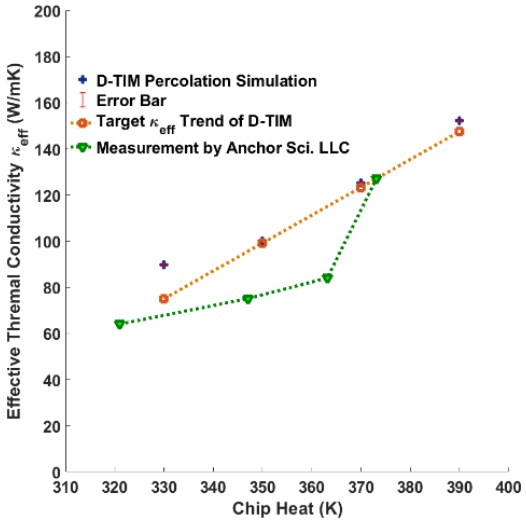

Fig.5: Simulation result of the effective thermal conductivity, using the optimized parameters by genetic algorithm.