

**Controlled formation of ball-milled carbon quantum dots via optimized graphite structures
by numerical simulation**

Sonia Lu Tai,¹ Kelly Qi Wang,¹ Ryan Taoran Wang,^{2,*} Gu Xu,¹ Alex Fan Xu,^{3,*}

¹ Department of Materials Science and Engineering, McMaster University, 1280 Main St. W,
Hamilton, ON L8S 4L8, Canada

² Energy Materials and Optoelectronics Unit, Songshan Lake Materials Laboratory, China
Academy of Sciences, Dongguan 523808, China

³ State Key Laboratory for Artificial Microstructure and Mesoscopic Physics, School of Physics,
Frontiers Science Center for Nano-optoelectronics, Collaborative Innovation Center of Quantum
Matter, Peking University, Beijing 100871, China

*Correspondence: wangtaoran@sslslab.org.cn; xufan@pku.edu.cn

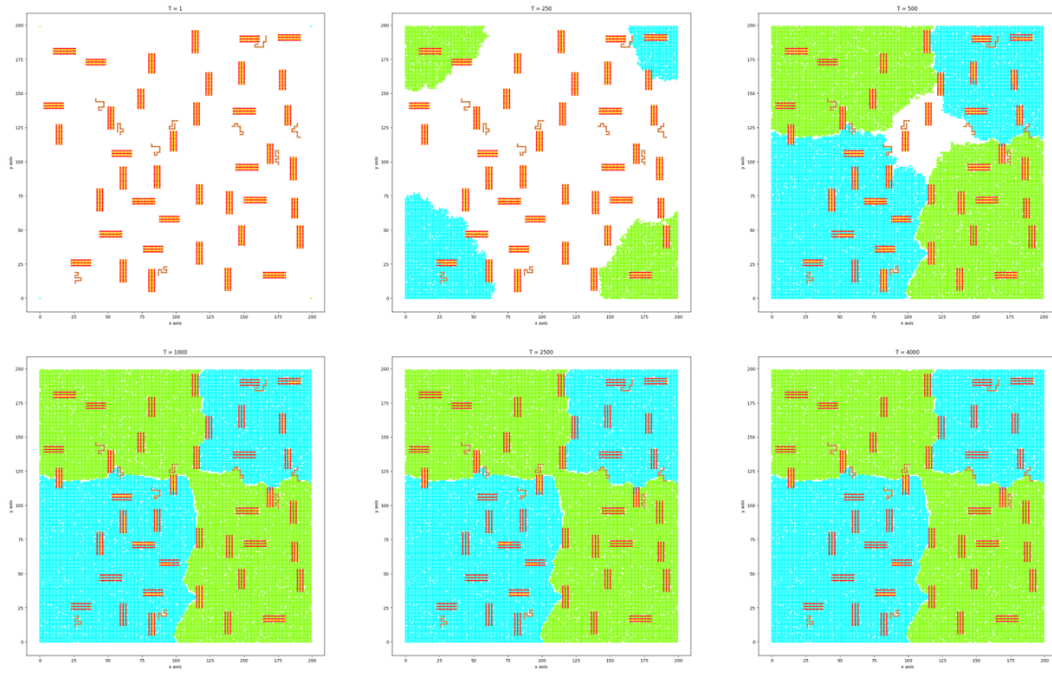


Figure S1. The simulation results of coal particles with layer number $n=5$ under shear stresses at iteration number T of 1, 250, 1000, 1000, 2500, 4000, respectively.

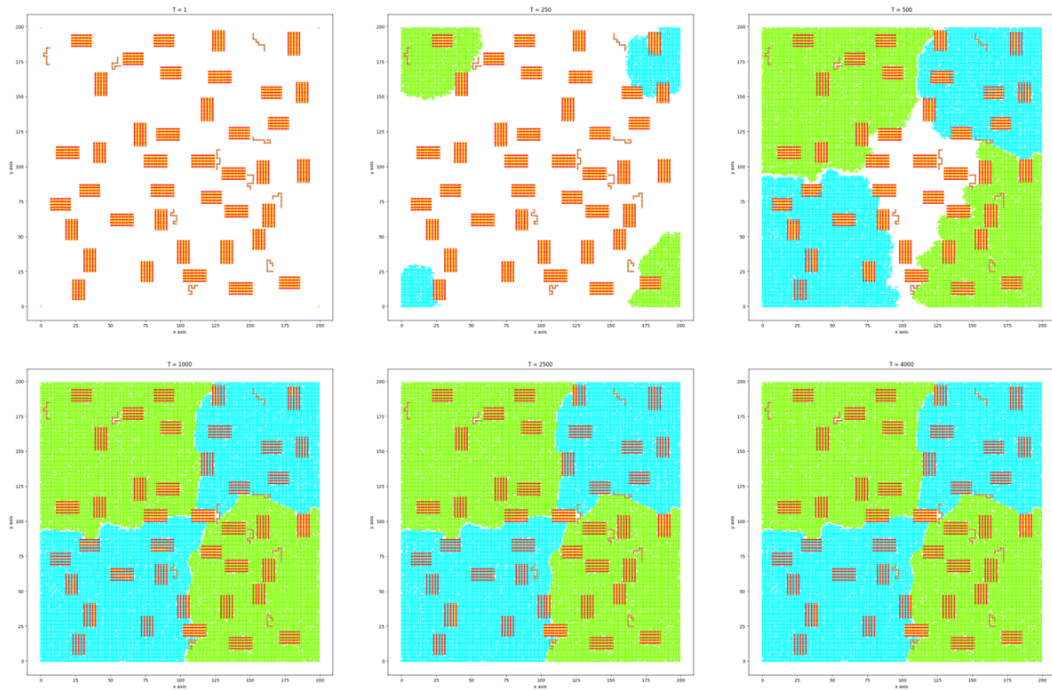


Figure S2. The simulation results of coal particles with layer number $n=9$ under shear stresses at iteration number T of 1, 250, 1000, 1000, 2500, 4000, respectively.

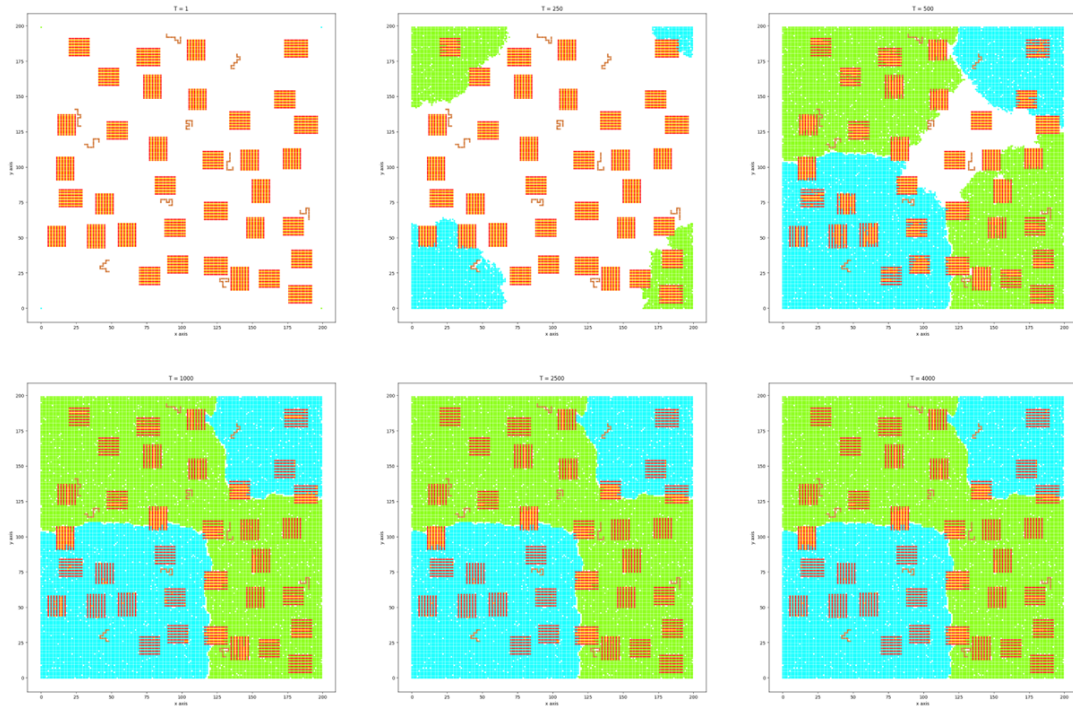


Figure S3. The simulation results of coal particles with layer number $n=13$ under shear stresses at iteration number T of 1, 250, 1000, 1000, 2500, 4000, respectively.

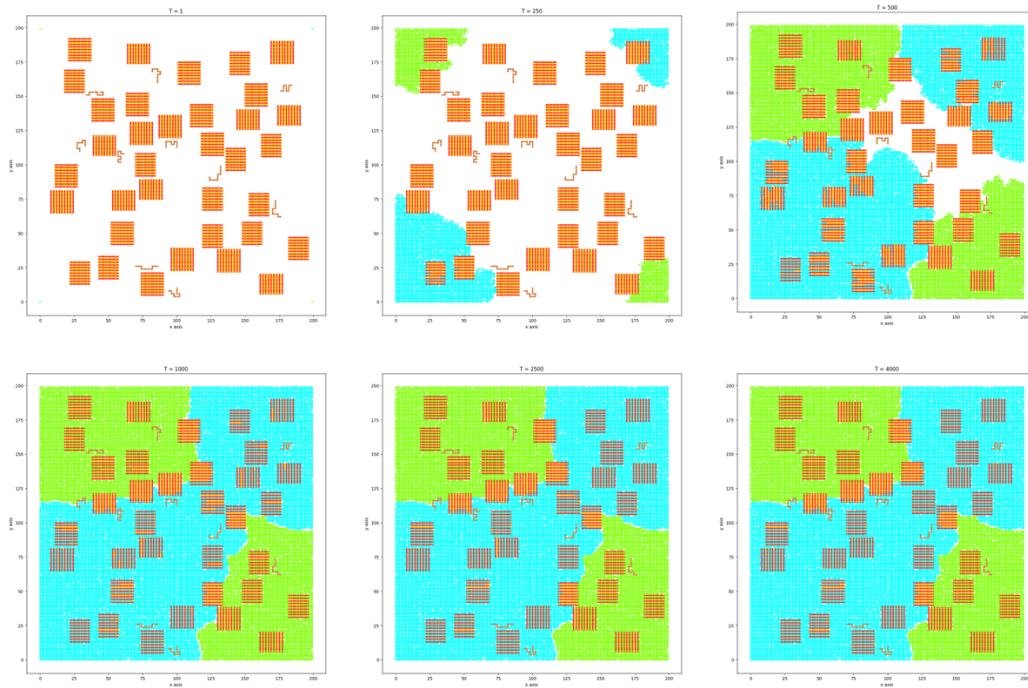


Figure S4. The simulation results of coal particles with layer number $n=17$ under shear stresses at iteration number T of 1, 250, 1000, 1000, 2500, 4000, respectively.

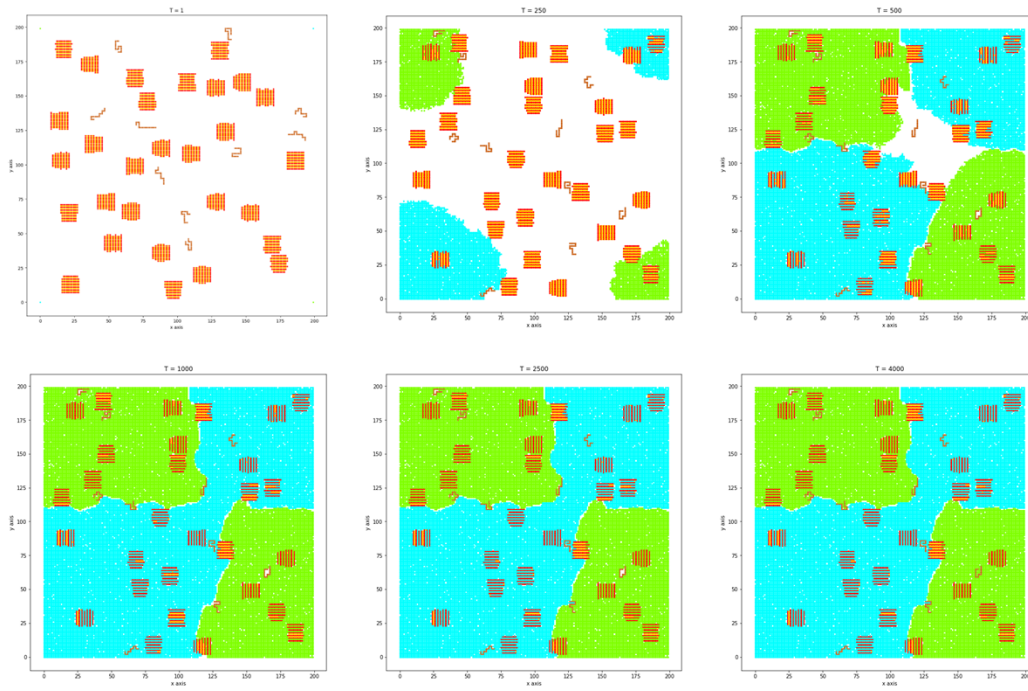


Figure S5. The simulation results of coal particles with lateral length $L=12$ under shear stresses at iteration number T of 1, 250, 1000, 1000, 2500, 4000, respectively.

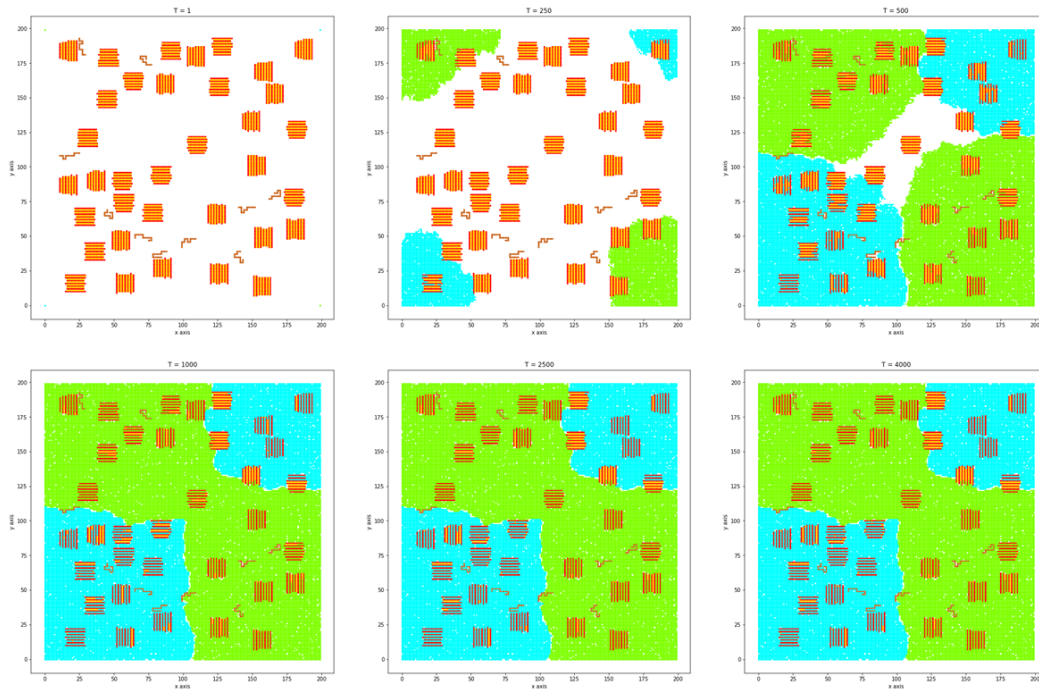


Figure S6. The simulation results of coal particles with lateral length $L=14$ under shear stresses at iteration number T of 1, 250, 1000, 1000, 2500, 4000, respectively.

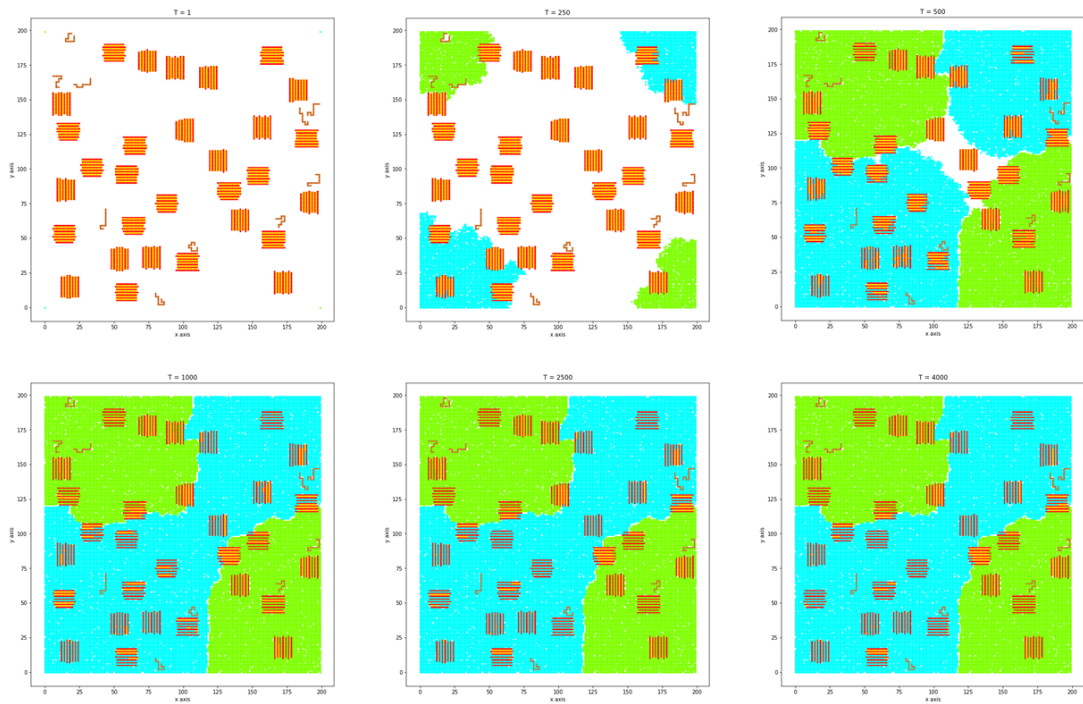


Figure S7. The simulation results of coal particles with lateral length $L=16$ under shear stresses at iteration number T of 1, 250, 1000, 1000, 2500, 4000, respectively.

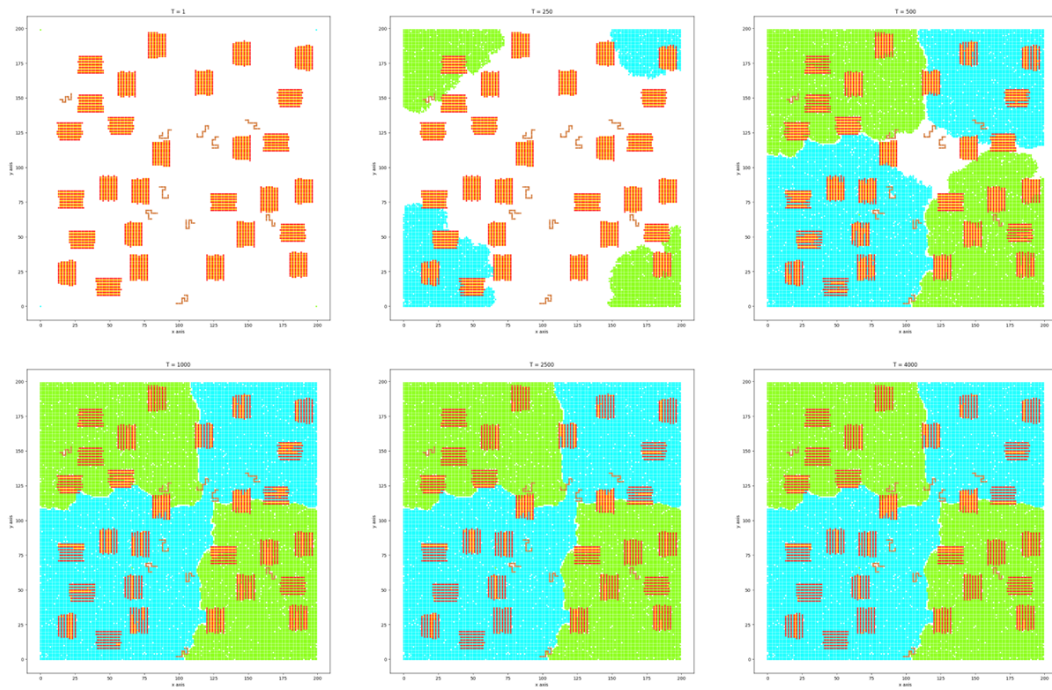


Figure S8. The simulation results of coal particles with lateral length $L=18$ under shear stresses at iteration number T of 1, 250, 1000, 1000, 2500, 4000, respectively.