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Molecular dynamics of heat pulse propagation in single and multi wall nanotube TAEJIN KIM, PhD Student, Material Science Program, MOHAMED OSMAN, Professor, The School of Electrical Engineering and Computer Science, CECILIA RICHARDS, DAVID BAHR, ROBERT RICHARDS, Associate Professors, The School of Mechanical and Materials Engineering — Molecular dynamics simulations have been used to investigate the nature of heat pulse propagation through single and multi wall nanotube. For the comparison, these simulations were carried out on armchair nanotube, (5,5) and (10,10), zigzag nanotube, (10,0) and multi wall nanotube, which is built by (5,5) and (10,10). All of the simulations were run at 0K, and the length of the pulse was 1ps. Results have shown that the heat pulse excites a variety of phonon modes. The speed of leading wave packets of single nanotube is about 20Km/sec and this is corresponding to speed of sound in longitudinal acoustic (LA) mode. The speed of following wave packets is about 16Km/s and this value is corresponding to twisted (TW) phonon modes. The strongest wave packets propagate together with the speed of 12Km/s and this speed corresponds to the second sound waves. In multi wall nanotube, the overall phonon modes show the interaction between each single nanotube phonon modes.

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