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Stability and Graphitization of Carbon Nanotube Arrays at high Temperature and Pressure[1] FRANCESCO COLONNA, EVERT JAN MEIJER, Van' t Hoff Institute for Molecular Sciences, University of Amsterdam, Nieuwe Achtergracht 166, 1018 WV Amsterdam, The Netherlands, ANNALISA FASOLINO, Institute for Molecules and Materials, Radboud University Nijmegen, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands — We investigated the effects of high temperatures and pressures on carbon nanotube arrays, focusing on structural changes like collapse, polymerization and graphitization. Building on our earlier work on graphite[1], we addressed those topics by means of Monte Carlo simulations, using a state-of-the-art bond-order potential (LCBOPII) capable to make and break bonds and to account correctly for the long-range interaction between graphitic structures. The structural changes and the graphitization mechanism appear to depend on temperature, pressure, and on the radius of the nanotubes. We discuss the possible transformation mechanism for temperatures up to 4000K and pressures up to 20GPa. [1] F. Colonna et al, Phys. Rev. B. 80, 134103 (2009).

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