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**Atomistic simulation of the laser fragmentation of single wall carbon nanotubes** HARALD JESCHKE, Institut für Theoretische Physik, Universität Frankfurt, Robert-Mayer-Str. 8-10, 60054 Frankfurt, Germany, ALDO ROMERO, Advanced Materials Department, IPICYT, Camino a la presa San José 2055, CP 78216, San Luis Potosí, SLP, México, MARTIN GARCIA, Universität Gesamthochschule Kassel, Fachbereich Physik, Theoretische Physik, Heinrich-Plett-Str. 40, 34132 Kassel, Germany, ANGEL RUBIO, Departamento de Física de Materiales, Facultad de Químicas, Universidad del País Vasco, 20018 San Sebastián/Donostia, Spain — Femtosecond laser induced structural changes in single wall carbon nanotubes (SWNTs) are investigated by extensive molecular dynamics simulations on time dependent potential energy surfaces. The damage threshold of the SWNT is shown to depend on the chirality of the tube, on its diameter as well as on the laser pulse parameters. For the studied laser parameters, zigzag SWNTs are shown to be more stable with respect to laser excitation than armchair SWNTs. The diameter dependence of the thresholds for structural modification turns out to be nonmonotonic, suggesting the possibility of selectively evaporating SWNTs from nonhomogeneous tube bundles.

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