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Melting and Premelting of Carbon Nanotubes[1] KAIWANG ZHANG, Xiangtan University, G. MALCOLM STOCKS, JIANXIN ZHONG, Oak Ridge National Laboratory — We report results of molecular dynamics simulations of melting and premelting of single-walled carbon nanotubes (SWNTs). We found that the traditional critical Lindemann parameter for melting of bulk crystals is not valid for SWNTs. Using the much smaller critical Lindemann parameter developed for melting of nanoparticles as a criterion, we show that the melting temperature of perfect SWNTs is 4800K. We further show that Stone-Wales defects in a SWNT significantly reduce the melting temperature of atoms close the defects, resulting in premelting of SWNTs around the defects at 2600K.

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