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Thermal expansion, elastic modulus and phase transition of carbyne: A stochastic model of chemical bonds distribution

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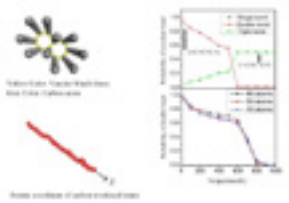
In the present work, we develop a powerful Monte Carlo algorithm of the carbon nanowires ordered into 3D hexagonal array. A new routine has been developed to probe the phase transition between the alpha and beta carbyne based on the chemical bond and atomic distributions. Our model confirms that the cumulene is the more preferable phase at low temperatures, but it is switched into polyvne phase at high temperatures. The bond softening temperature across Peierls transition is observed at 480 K. The higher Peierls transition temperature is observed in the presence of interstitial doping despite the transition temperature shows length-independence. The elastic modulus of the carbon chains is 1.7 TPa at 5 K and the thermal expansion is +70 μ K-1 at 300 K via. monitoring the collective atomic vibrations and chemical bond distributions. Thermal fluctuation in terms of heat capacity as a function of temperatures shows that the melting point is around 3800 K. The carbon atoms along the carbon nanowire arranged in relaxed state is unveiled at the end.



Biography

C H Wong has his expertise in Monte Carlo simulation and ab-initio calculation in Material Science. He has passion in searching for 300 K superconductors. He admitted in an experimental physics group and was trained to conduct AC calorimetry in the resolution better than 5 decimal places during his Doctoral degree in Hong Kong. He made contributions in capturing tiny superconducting signals in nanostructured materials and also discovered more fundamental physics of superconductors based on the ultra-weak heat capacity anomaly. After he graduated in 2015, he explores in theoretical condensed matter physics as a Post-doctoral Researcher in Russia, in order to design high temperature superconductors from theoretical point of view. He has constructed a stochastic model for carbon nanowire carrying extremely large Debye frequency and proposes the algorithm towards stabilized carbon nanowires array.

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