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Stochastic model of carbon nanowires array

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Abstract:

In the present work, a Monte Carlo algorithm of the carbon chains in form of 3D hexagonal array is developed. A new routine is proposed to probe the phase transition between the alpha and beta carbyne according to the chemical bond and atomic distributions. Our simulation provides evidence that the beta phase is more energetic preferable at low temperatures while the carbon chains prefer to transit into alpha phase at high temperatures. The bond softening temperature occurs at ~480K. The larger bond softening temperature is observed in the presence of interstitial doping. The predicted elastic modulus of the carbon chains is 1.7TPa at 5K and the thermal expansion is +70μ K^{-1} at 300K via monitoring the collective atomic vibrations and bond distributions. Thermal fluctuation in terms of heat capacity as a function of temperatures shows that the melting point is around 3800K. The carbon atoms along the carbon nanowire occupied in relaxed state is displayed at the end.

Monte Carlo method:

All carbon atoms are connected by C=C and separated by 134pm as the initial condition at each temperature. The selected atom following metropolis [1] selection may move to the new dx, dy, dz and also amend the type of bond based on the energy minimization. The inter-chain distance is 0.3nm.

$$H = e^{-T/T_{bj}} \sum_{m=1}^{M} \sum_{n=1}^{N-1} \left| E_{m,n,j} e^{-\frac{r_{m,n} - r_{m,n,j}^{eq}}{0.5 r_{m,n,j}^{eq}}} - E_2 \right| + e^{-T/T_{bj}} \sum_{m=1}^{M} \sum_{n=1}^{N-1} J_A \left(\cos\theta + 1 \right)^2 - 4\varphi \left[\sum_{n,m} \left(\frac{\sigma}{r}\right)^6 - \left(\frac{\sigma}{r}\right)^{12} \right] + W_{external}$$

$$dz = \pm 3.8x10^{-12} p\sqrt{T} \qquad dx = dy = \frac{kT}{\left(E_1 + E_2 + E_3 \right) / 3} dz$$

For example, $r_{12,8,1}$ refers to the equilibrium position of 12th atom along 8th chain which is connected by single bond. The breakdown temperature of the covalent bond T_{bj} is found by $E_j = kT_{bj}$ where k is Boltzmann constant and J_A = 1x10^{-18}J. σ = 1.23x10^{-10}m, φ = 8.1x10^{-23}J, θ is the pivot angle between the three nearest atoms, W is the mechanical work done with the parallel force F_z =8.1nN and p is the frictional factor which is a random number between 0 and 1. N is the total number of atoms along the chain while M is the total number of chains. The bond selection is controlled by Octet rules at equilibrium. [2]

Figure 1: (a) The cross section of the hexagonal carbyne. (b) The atomic arrangement of the carbon at initial condition. (c) Simulation results of the relaxed carbon nanowire.

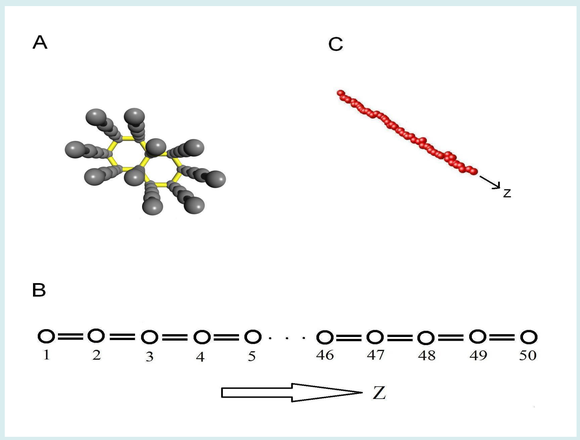


Figure 2: The probability of retaining double bonds reduces upon heating. More single and triple bonds are formed upon heating due to Boltzmann excitation across Peierls transition.

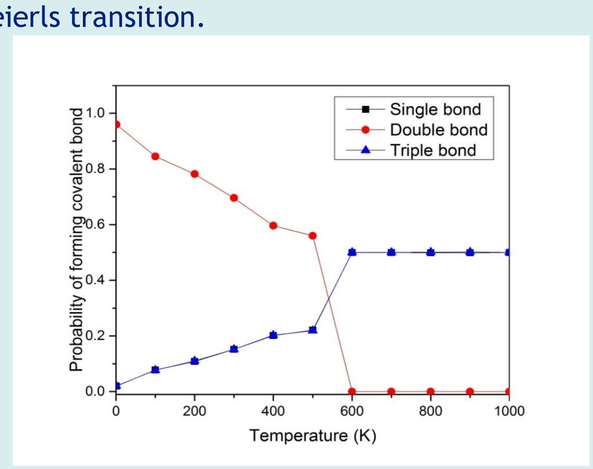


Figure 3: The Peierls transition temperature is increased by the decrease of MPF because more thermal energy is required to rearrange the atomic positions

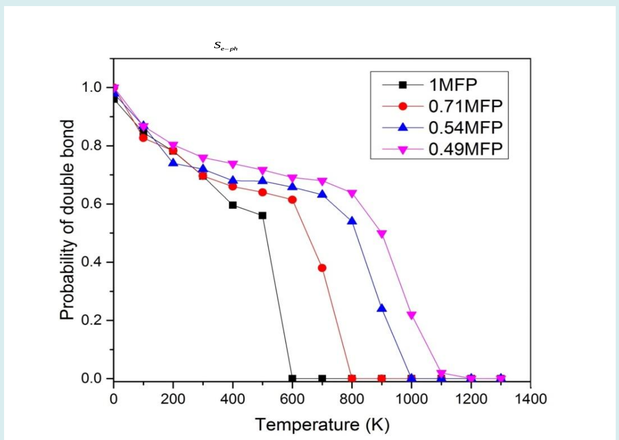


Figure 4: The Peierls transition temperature does not influenced by chain length because the atomic mean free path (0.71MPF) remains unchanged.

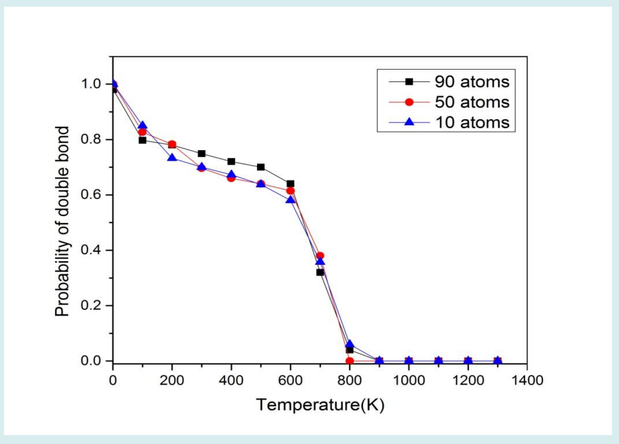
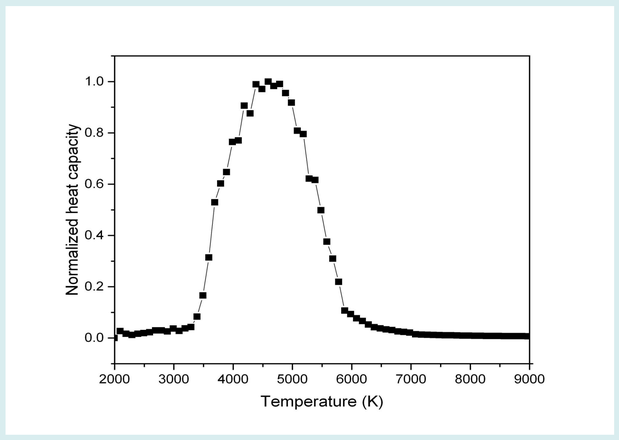


Figure 5: The melting point of the carbon nanowire is in the range of few thousands Kelvin. The anomaly is activated at 3500K and returns to zero above 6000K.



References:

[1] V. V. Prudnikov , etal, Investigation of the effects of aging and temperature dependence of the transverse rigidity of a system in the two-dimensional XY model, The Physics of Metals and Metallography, Volume 115, Issue 12, pp 1186-1193 (2014)

[2]: C.H.Wong*, E.A. Buntov, V.N. Rychkov, M.B. Guseva, A.F. Zatsepin, Simulation of chemical bond distributions and phase transformation in carbon chains, Carbon, Volume 114, Pages 106-110 (2017)