Influence of the force field on the height of energy barrier for carbyne-graphene nanoelements break

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Introduction

Carbyne (a linear form of carbon) and carbyne-graphene nanoelements (graphene sheets linked by a carbyne chain) are the promising materials for carbon based nanoelectronics. The key property that affects the practical use is their thermomechanical stability and lifetime under the action of force fields. A key factor that controls the value of these properties of carbyne is sensitivity of the energy barrier height for chain break from the magnitude of the applied force. The work is aimed at studying the relationship between the work required to break the chain and the level of the force field.

Classical Theory

According to Zhurkov's classical theory, the relationship between the work required to break the chain and the applied force must be linear, and the γ will make sense of the activation volume.

$$\frac{\tau}{\tau_0} = \exp\left[\frac{E_b}{k_B\, T}\right]$$

$$E_b = E_0 - \gamma F_f -$$
current energy barrier height, and E_0 *–bond energy*

According to the research findings, this dependence for carbyne-graphene nanoelements is essentially nonlinear.

Method

Nonlinear character of dependency between energy barrier height E_b and applied force F_f is considered. Deformation dependencies for E_b are found from DFT-calculations. Approximation of these data with Morse-type curve allowed to find the analytical relationship between the contact bond break work and the applied force without instability zone (1) and considering it (2):

(1)

$$E_b = E_{b\,max}\sqrt{1 - \frac{F_f}{F_{un}}}$$

(2)

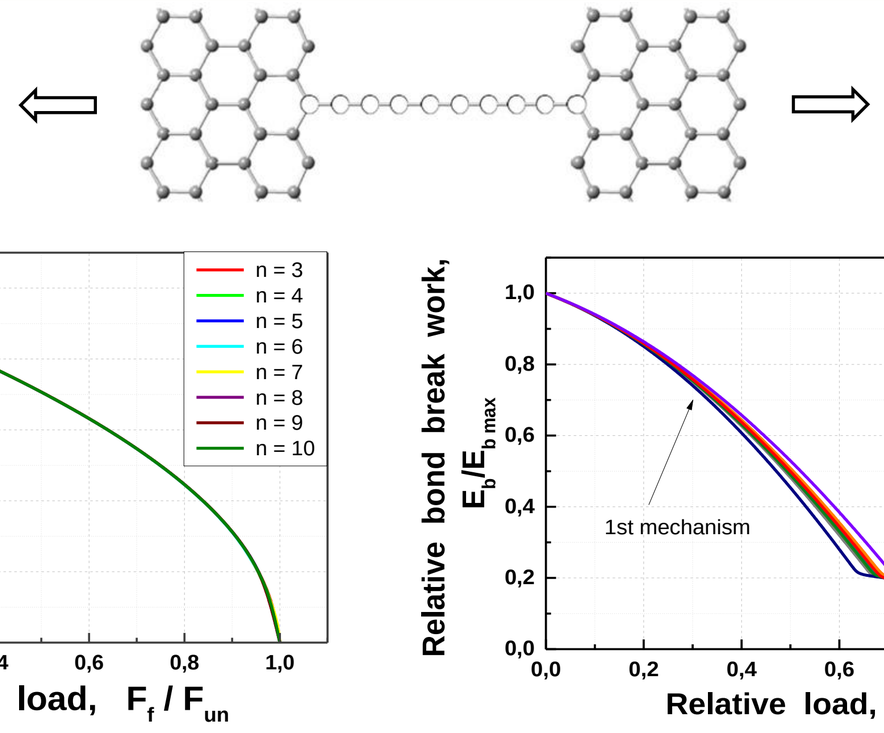
$$E_b = F_{\text{un}}\sqrt{1 - \frac{F_f}{F_{\text{un}}}} - \frac{1}{2}\frac{(u_R - u_{\text{un}})(F_{\text{un}} + F_R)}{(F_{\text{un}})^2}{F_f}^2$$

$$F_R = \sqrt{{F_{\text{un}}}^2 - \alpha {F_f}^2} \qquad 1^{\text{st}}\text{ mechanism}$$

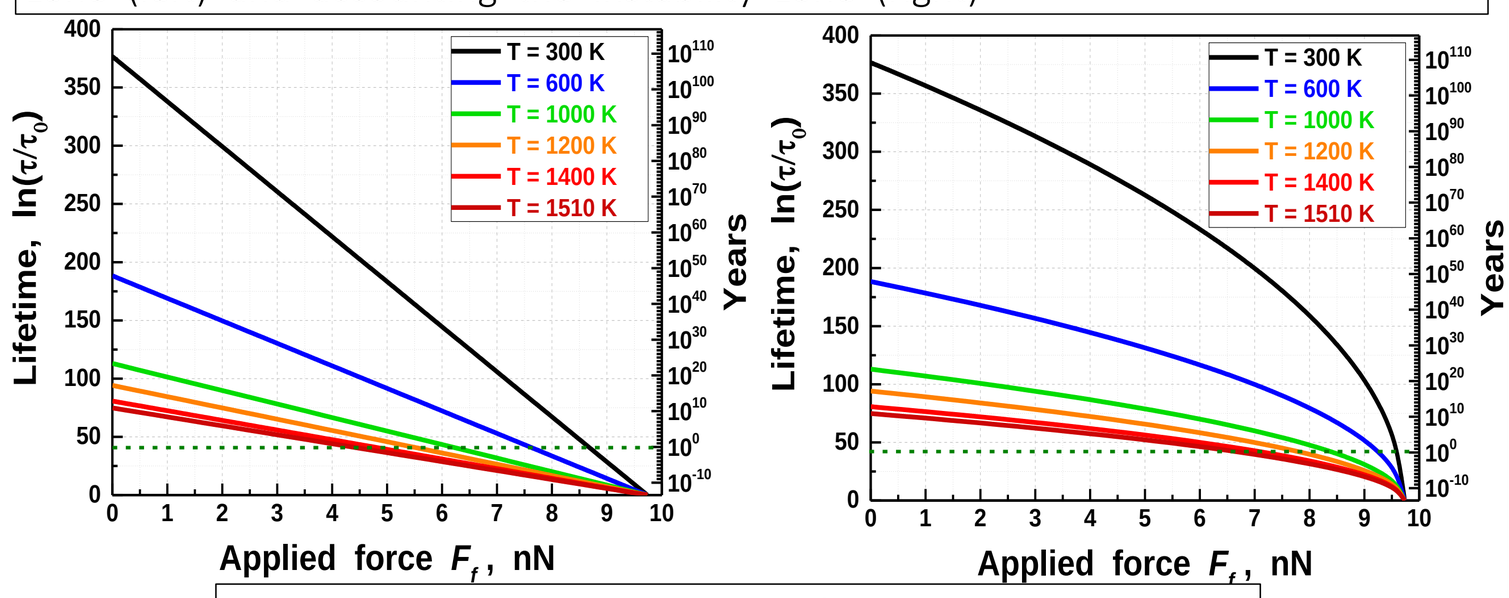
$$\alpha = 1 - \left(\frac{F_{R\,\min}}{F_{\text{un}}}\right)^2$$

$$E_b = -\frac{3\,F_{\text{un}}}{4} - F_{\text{un}}\,(-2\,\beta + \beta^2) \qquad 2^{\text{nd}}\text{ mechanism}$$

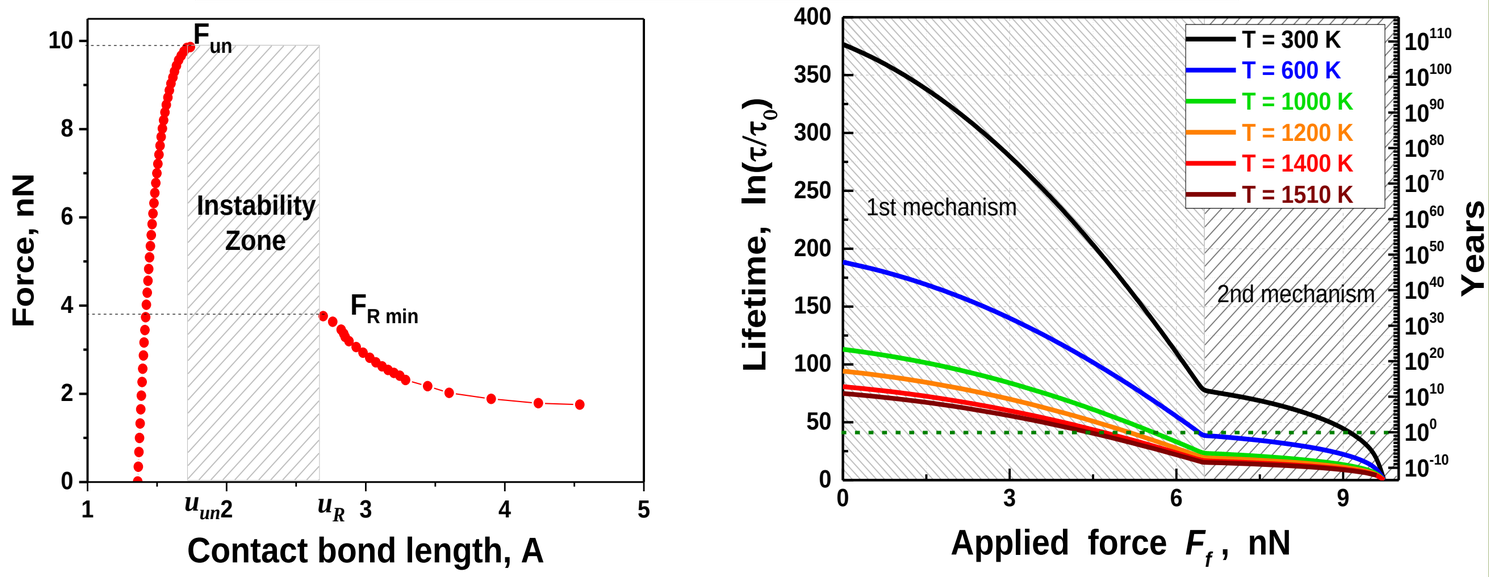
$$\beta = \left(\frac{1}{2} + \frac{1}{2}\sqrt{1 - \frac{F_f}{F_{\text{un}}}}\right)$$



Dependence between bond break energy and applied force without instability zone (left) and accounting the instability zone (right)



Carbyne-graphene nanoelement lifetime prediction:
left – Zhurkov theory (linear dependency),
right – non-linear dependence.



Carbyne-graphene nanoelement lifetime prediction accounting the instability zone:
left – deformation curve for nanoelements with 10-atom carbyne chain,
right – lifetime prediction.

Conclusions

1. For nanoobjects dependency between energy barrier height and applied force is essentially nonlinear.
2. Existence of instability zone is a characteristic feature of carbyne-graphene nanoelements (CGN) deformation dependency. Thus it results two mechanisms of contact bond break in CGN and, consequently, two regions on lifetime dependency.
3. Classical Zhurkov's model can`t describe effects inherent in nanomaterials and CGN.

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