Synergy of the effect of temperature and force field on stability and lifetime of nanosized elements consisting of one- and two-dimensional nanostructures

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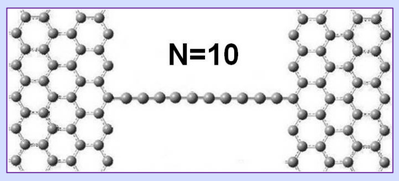
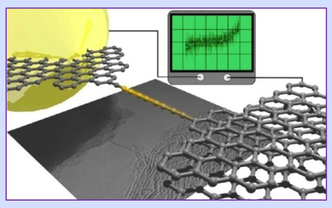
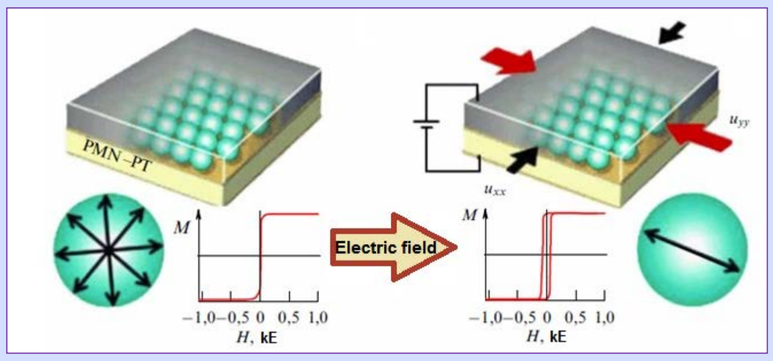
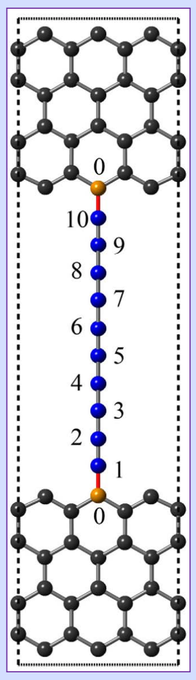




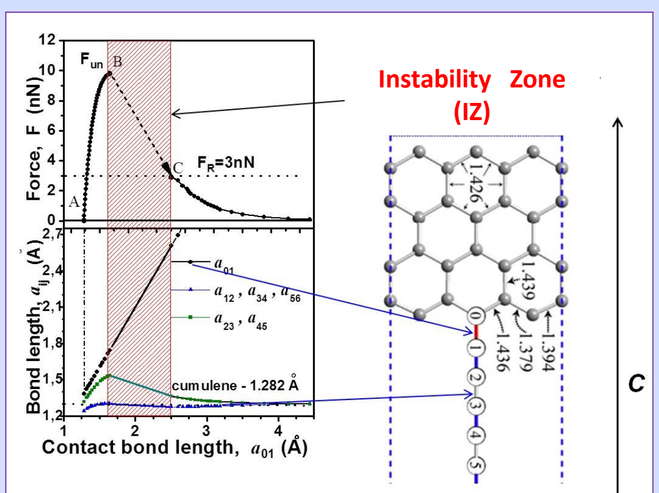


Carbyne-graphene nanoelements (CGNs) are currently considered as one of the main components of all-carbon-based nanodevices. These are ***graphene sheets joined by a monatomic chain of carbon atoms***. Current trend of transition to practical use of nanoelements requires to study mechanisms that govern their lifetime under conditions ***of combined action of such factors as temperature and mechanical load***. This is crucially important for straintronics elements, as they involve governing the functional properties of nanoelements by deforming them. Failure mechanism at these conditions is a fluctuation-induced interatomic bond break under the action of a force field.

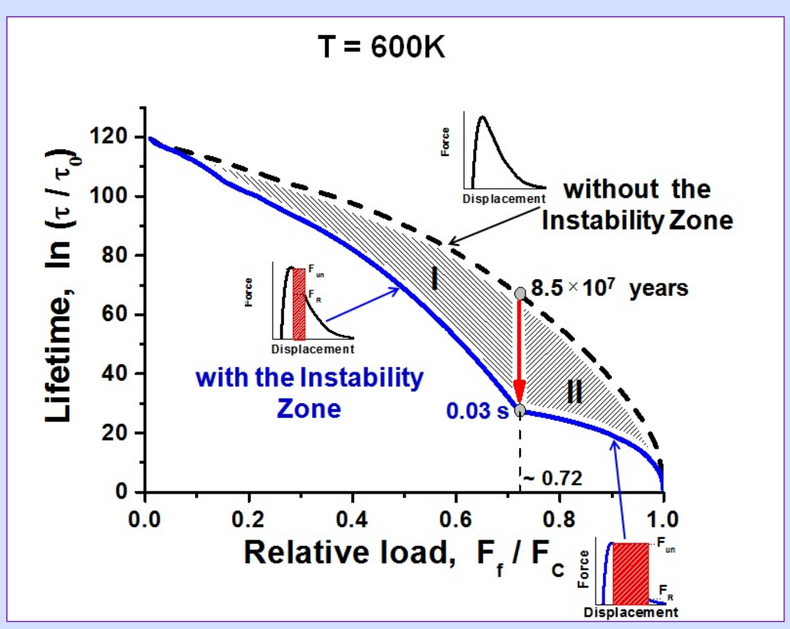
The task of the report is to show that the synergy of temperature and force field is a specific feature of the mechanism that governs the lifetime of nanosized elements, consisting of a combination of one- and two-dimensional structures



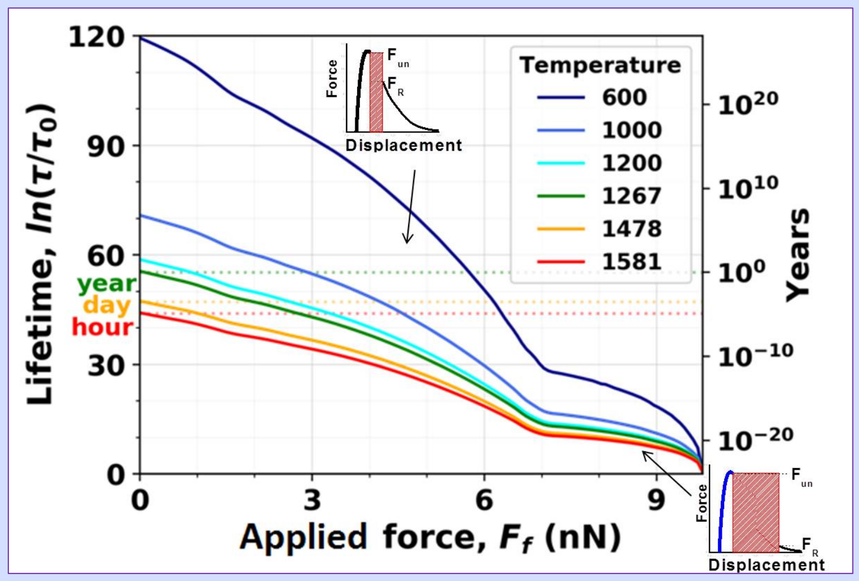
Instability Zone as a reason for synergy



Dependence of the force **F**, acting in a contact bond, on its length, a_{01}, as well as accompanied changes in the lengths of atomic bonds inside of the carbyne chain.



CGN life-time prediction for some temperatures



Approximation dependences of CGN-10 lifetime:

$$\ln\frac{\tau}{\tau_0}=\frac{E_0}{K_BT}\cdot\sqrt{1-F^*}$$ - without IZ

$$\ln\frac{\tau}{\tau_0}=\frac{E_0}{K_BT}\cdot\left[\sqrt{1-F^*}-\frac{1}{4}\cdot\left(\left\{1+\sqrt{1-\sqrt{1-\alpha\cdot\left(F^*\right)^2}}\right\}^2-1\right)\right]$$ - with IZ (region I)

$$\alpha=1-\frac{F_{R\min}^2}{F_{un}^2}$$

is the *basic* parameter characterising IZ width and, respectively, the effect of synergy

$F^*=\frac{F_f}{F_{un}}$ **is the relative load**

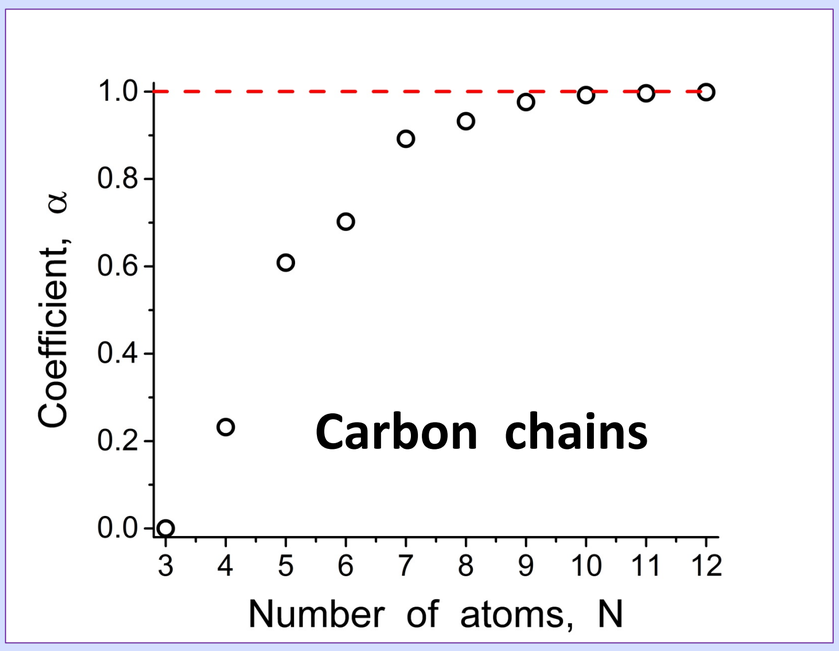
F_f **is the applied force**

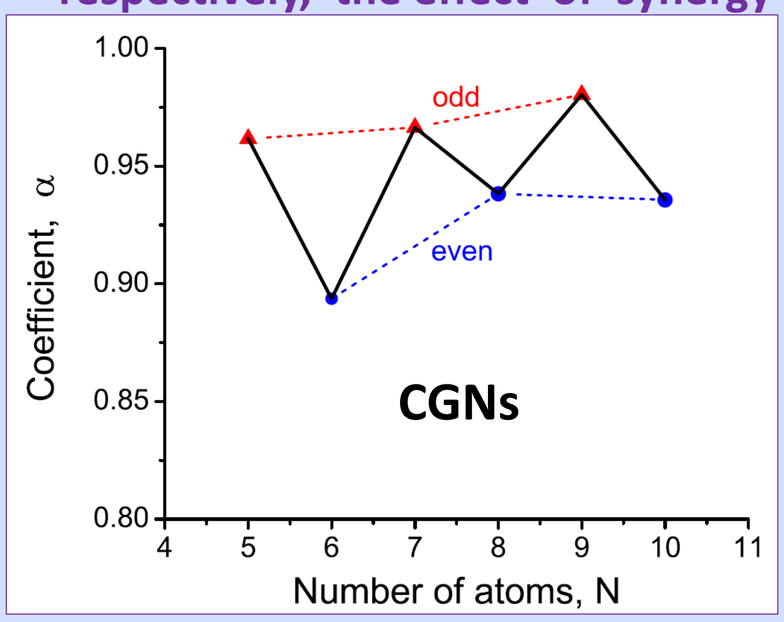
F_{un} **is the force of instability**

$F_{R\min}$ **is the minimum value of IZ low boundary F_R**

E_0 **is the contact bond energy**

K_B **is the Boltzmann constant**





Conclusions

1. **IZ** is a key feature of the behaviour of nanosystems under mechanical stresses. This has a ***crucial effect*** on CGNs' lifetime (decrease from ***millions of years*** to ***ms***).
2. **IZ** is the reason for ***synergism*** of the effect of both temperature and mechanical load on the level of thermo-mechanical stability and life-time of CGNs.
3. Life-time of a carbyne nanoconductor is ***sufficient*** for application at temperatures not higher than 1000K and loads not higher than 30% of it strength.

References

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