International Conference

on Differential Equations, Mathematical Physics and Applications

BOOK of ABSTRACTS

October 17-19, 2017
Cherkasy, Ukraine

Organized by

Ministry of Education and Science of Ukraine

Bohdan Khmelnytsky National University of Cherkasy

Vasyl' Stus Donetsk National University

Institute of Mathematics of NAS of Ukraine

Institute of Applied Mathematics and Mechanics of NAS of Ukraine

G.V. Kurdyumov Institute for Metal Physics of NAS of Ukraine

Physical and Technical Institute of NAS of Belarus

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where: $p(k,tt) = \frac{\gamma(k,tt)}{\Gamma(k)}$, $\Gamma(k) = \gamma(k,+\infty)$, $\gamma(k,tt) = \int\limits_0^{tt} x^{k-1}e^{-x}dx$.

7. In the case $G >> 1$ we can limit ourselves to the formation and growth of single pore. Then we suggest some heuristic considerations: The time to reach a certain probability P with the failure criterion $X_{threshold}$, approximately equal: $tt \approx T_1 + T_2$, were T_1 - waiting time of pore nucleation, T_2 - growth time of the single pore. $T_1 = -ln(1-P), T_2 \approx \frac{f(X)}{G}$. If we make the transition to dimensional units, then:

$$t \approx (-ln(1-P) + \frac{f(X)}{\frac{V}{\nu L^3}})\frac{1}{\nu L^2} \approx \frac{-ln(1-P)}{\nu L^2} + f(X)\frac{L}{V}. \quad (4)$$

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First principles DFT study of structural, electronic and mechanical properties of two-dimensional nitrogen monolayers

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The single-bonded 2D nitrogen allotropes of the honeycomb (A7) and zigzag sheet (ZS) topology are calculated by density functional theory (DFT). The optical, thermodynamic and elastic properties of these 2D sheets have been calculated for the first time. Phonon dispersion calculations have justified these structures as vibrationally stable 2D materials. The IR spectroscopy can not be useful in the characterization of the studied materials, while the Raman spectroscopy can be effectively applied for the experimental spectral identification. (the calculated IR intensity completely failed for detection). The UV absorption spectra prediction demonstrates complete opacity of the A7 and ZS monolayers to the UV irradiation above 9 and 6 eV (140 and 210 nm), respectively. Thus, the studied materials are predicted to be transparent to visible light. Calculations of NMR magnetic shielding tensors indicates that the electron density arrangement around the nitrogen nuclei in the studied polynitrogen sheets is much denser compared to the N2 molecule. The elastic constants reveal a robust mechanical stability of the studied 2D nitrogen allotropes and the calculated Young moduli values are only twice as lower than that of the graphene molecule.