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

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Suvorova I.G., Investigation the hydrodynamics of flows in channels of complex geomet-	
$ric\ forms$	84
Trofymenko O.D., Convolution equations and two-radii theorems for solutions of linear	
elliptic equations with constant coefficients in the complex plane $\ldots \ldots \ldots$	85
Vorobyova A., Group analysis of wave equation with special right-hand side	87
Yehorchenko I., Relative differential invariants and invariant equations equations	88
STOCHASTIC DIFFERENTIAL EQUATIONS	90
Borysenko O.D., Borysenko D.O., Global solution to stochastic logistic equation	90
Buchak Kh.V., Sakhno L.M., Investigation of properties of time-changed Poisson processe Doobko V.A., Derivation of the diffusion equation in random fields from the special	s 91
$Langevin \ equation \qquad \ldots \qquad $	92
Ivanov I.L., Correlation results for some foreign exchange markets	93
Kozachenko Yu.V., Petranova M.Yu., Simulation of the Ornstein-Uhlenbeck process \ldots	94
Lohvinenko S.S., Parameters estimation in fractional Vasicek model	95
Osypchuk M.M., Portenko M.I., Jump theorem and its applications	97
Pashko A., Vasylyk O., Accuracy of simulation of fractional Brownian motion in	
$L_p([0,T])$ and $C([0,T])$	98
Pryhara L.I., Shevchenko G.M., Regularity of solution to the wave equation with a	
coloured stable noise	100
Radchenko V.M., Averaging principle for heat equation driven by general stochastic	
measure	101
Ralchenko K.V., Statistical inference for fractional Ornstein–Uhlenbeck process	102
Ralchenko S.A., Existence and uniqueness of solutions to stochastic differential equa-	
tions driven by fractional Brownian field	103
Rozora I.V., Some properties of impulse response function	105
Sakhno L.M., CLT for quadratic forms for random fields with tapered data and asymp-	
totic properties of minimum contrast estimators	106
Shklyar S., Ralchenko K.V., Mishura Yu., Maximum likelihood estimation of the drift	105
slope of a Gaussian process	107
Tsukanova A.O., On comparison theorem for the Cauchy problems to neutral stochastic	107
integro-differential equations	107
Yamnenko R.E., Yanevych T.O., Some properties of random processes from Orlicz	110
spaces of exponential type	110
MATHEMATICAL PROBLEMS OF PHYSICS AND MATERIALS SCIENCE	111
Auzinger W., Adaptive integration of large linear systems of Schrödinger type with time-	
dependent coefficients using Magnus-type methods	111
Bezpalchuk V., Kozubski R., Gusak A., Simulation of the tracer diffusion and ordering	
kinetics in FCC structures - Stochastic Kinetic Mean-Field Method	112
Bhat A.P., Dhoble S.J., Rewatkar K.G., Effect of rare earth doped metamatrial towards	
the antenna miniaturisation and substrate primitive \ldots \ldots \ldots \ldots \ldots \ldots	113
Bobrov O., Pasichnyy M., Gusak A., Size effect on distributions of times to failure and	
times to transformations	114
Bondarchuk S.V., Minaev B.F., First principles DFT study of structural, electronic and	
mechanical properties of two-dimensional nitrogen monolayers	115
Borisenko A., Nominal vs. active supersaturation of solutions	116
Gavrilik A.M., Kachurik I.I., Hermitian Hamiltonian built from Non-Hermitian posi-	
tion/momentum operators, and deformed oscillators	117
Gokhman O., Terentyev D., Kondrea M., Investigation of the post-irradiation annealing	1 1 F
on the defect structure of tungsten	117

where: $p(k,tt) = \frac{\gamma(k,tt)}{\Gamma(k)}, \ \Gamma(k) = \gamma(k,+\infty), \ \gamma(k,tt) = \int_{0}^{tt} x^{k-1} e^{-x} dx.$

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:

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