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Computational Analysis and Finite Element Modelling of Nanoscale Ripples in Graphene and Thermomechanical Effects

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Abstract *– The relaxed state of graphene nanostructures due to externally applied tensile stress along both the armchair and zigzag directions are analyzed in detail. The results, obtained with the Finite Element Method (FEM), demonstrate that the amplitude of ripple waves in such nanostructures increases with temperature. Details of the multiscale multiphysics computational procedure developed for this analysis are also provided.*

Key words – nanostructures, modelling, coupled processes, computer-aided design, nanotechnological applications.

I. Introduction

Graphene, a hexagon structure where the atomic layer of carbon atoms are arranged in a honeycomb lattice, is the thinnest material that can be found in the nature. It is poised to make a new breakthrough in nanotechnology due to the high mobility of charge and the potential interest to control its electronic properties by several different mechanisms such as gate controlled electric fields, magnetic fields and engineering the electromechanical properties via the pseudomagnetic gauge fields (see, e.g., [1] and references therein).

However, by now it is well known that the graphene sheets are not perfectly flat. They exhibit intrinsic roughening such that the surface normal varies by several degrees and the out-of-plane deformations reach to nanometer scale, known as ripples. In this contribution, we apply the computer-aided design methodology, based on FEM, to analyze such ripples.

II. Mathematical Model

We present a model that couples the Navier equations including thermomechanical effects to the electronic properties of graphene-based nanostructures. We start with the total thermoelastic energy density associated to the strain for the two dimensional graphene

$$U_s = \frac{1}{2} C_{iklm}\ \varepsilon_{ik}\ \varepsilon_{lm} - \beta_{ik}\ \Theta(x,y)\ \varepsilon_{ik}\ \delta_{ik},$$

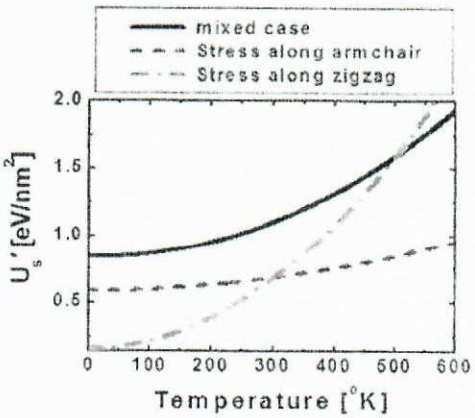
where C_{iklm} is the elastic modulus tensor of rank four, ε_{ik} is the strain tensor, β_{ik} is the stress temperature coefficients, Θ is the distribution of temperature in the graphene sheet that can be found by solving Laplace's equation for the temperature, assuming the Fourier law. As a result, we have to solve the coupled Navier equations for the graphene nanostructure. Ripples in graphene are described by an out of plane sinusoidal function on the sheet of graphene and we apply tensile edge stress along the armchair direction to induce the ripples so that the total edge energy per unit length is given by

$$Ue = \frac{1}{2}\tau_e\left(\frac{\partial u(x,0)}{\partial x}\right)^2 + \frac{1}{8}E_e\left(\frac{\partial u(x,0)}{\partial y}\right)^4,$$

where τ_e and E_e denote the edge stress and the elastic modulus of the edge along the armchair direction of the graphene sheet.

III. Computational Analysis and Modelling

We have developed a multiscale multiphysics computer-aided simulation technique, based on the Finite Element Method, to analyze thermomechanics of relaxed states of graphene nanostructures. Among other results, we will discuss the total thermoelastic energy density vs temperature (Fig. 1). Even though the optimal amplitude value of the ripple waves has been the same in all three cases studied here, the variation in the the total thermoelastic energy density is enhanced for the case of induced ripples due to applied tensile edge stress along zigzag direction (dashed-dotted line). This is due to the fact that the graphene sheet at one of the boundaries is connected to the heat reservoir that enhances the energy of the ripple waves along the y-direction. These differences affect also electronic properties of graphene nanostructures.



Conclusion

In this contribution we have analyzed thermomechanical behavior of nanoscale ripples in graphene by using the developed multiphysics FEM-based computational technique.

References

[1] *A. H. Castro Neto* et al, "The electronic properties of graphene", Rev. Mod. Phys. 81, 109, 2009.

Contents

Real-time Preprocessing Filtering of Input Data for Stereo-vision System with Vary in Time Cameras Distance 1
Ivan Tsmots, Andrii Shkodyn, Dmytro Peleshko

Commercial Content Support Method in the Electronic Business Systems 2
Victoria Vysotska, Lyubomyr Chyrun, Liliya Chyrun

Algorithm and Tool to Develop a Forest Map by Using GWR Model in R: Case Study for Ukraine 6
Myroslava Lesiv, Dmitry Schepaschenko, Olexander Stryamets, Zbigniew Nahorski

Algorithms for Hierarchical Circuit Clustering and Partitioning 8
Roman Bazylevych, Sergii Byelyayev

Applying Metagame Analysis for Solving Imperfect Information Games 11
Serhiy Liakhevych

Computational Analysis and Finite Element Modelling of Nanoscale Ripples in Graphene and Thermomechanical Effects 14
Roderick Melnik, Sanjay Prabhakar

Uncertainty of Greenhouse Gases Spatial Inventory: Power and Heat Production 15
Petro Topylko, Rostyslav Bun, Oleksandr Striamets, Olha Danylo

Development Adaptive Critic for Decision Support Systems 17
Volodymyr Lytvynenko, Olga Kozhuhivska, Andrey Fefelov

Development of Additional Element University Corporate Identity Based On Specialized Windows 7 Themes 19
Anastasiia Iakymovych, Yuliya Miyushkovych

Distributed Computing for Phase-Field Models 20
Rakesh Dhote, Roderick Melnik, Hector Gomez, Jean Zu

Effect of Thermal Characteristics on the Distribution of Temperature Field in the Object 21
Liubov Zhuravchak, Olena Kruk

Formation of the Consolidated Data Resource of Tourism Information 25
Pavlo Zhezhnych, Oksana Soprunyuk

Formation of the Encyclopedic Content 26
Pavlo Zhezhnych, Mariya Hirnyak

Forms of Fuzziness in Data and Knowledge Bases 27
Oleksandr Siedushev, Ievhen Burov

Geometric Transformations for the Map Image Superimposition with the Aerial Photograph 31
Victoria Sablina, Anatoly Novikov, Michael Nikiforov

Lexical and Statistical Aspects of V. Stefanyk's Idiolect Study 34
Ihor Kulchytskyj, Yuliya Danchevska

Logistic Functionally Model of Commercial Content Processing 36
Andriy Berko, Victoria Vysotska, Lyubomyr Chyrun

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