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Structural stability of a ring quantum dot

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Nanoobjects have wide applications and are actively studied. They are distinguished by unique electronic properties. Investigating their electronic properties is impossible without detailed information about their atomic structure. This paper presents an approach which allows predicting the stability of nano-ring using classical approximations. The proposed approach is used to study a single-layer nano-ring, which is essentially a quantum dot cut from a nanotube. Approaches based on machine learning methods are currently often used to solve similar problems. However, classical approximations have not lost their significance and prove useful in a number of cases. This paper introduces the Hooke force for the angular and the radial stabilization of nano-ring. This makes it possible to formulate conditions for the structural stability of a ring quantum dot.

Keywords: nanoobjects, nano-ring, Lennard-Jones potential, potential of two springs, Hooke forces, local oscillations, quantum dot.

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Introduction. Problem Statement

The work presents a modification of the widely known Lennard-Jones (LJ) potential for the case when the system has cylindrical symmetry and is located at small distances from the equilibrium position. For these conditions, the LJ potential can be replaced by the N -spring potential. The use of this potential is illustrated for the case $N=2$ (nanoring). In the case of studying a nanotube (using the N -spring potential with $N=3$), an additional equilibrium equation should be considered.

A nanoring is a system of model atoms for which the preservation of ring symmetry, stability of the radius, the value of interatomic distances and the balance of forces must be consistent with each other. If, for example, the LJ potential is used, then the main parameters of the nanoring model become the energy scale ε and the characteristic spatial scale σ . In the case of using the potential of two springs, we also have two parameters, and these are

already 2 elasticity coefficients. In this case, the problem is reduced to solving two mutually related equilibrium equations (in the radial and tangential directions). To obtain the appropriate solution, a computer program has been developed, which provides the solution of the equilibrium equations with simultaneous step-by-step comparison of intermediate results with the standard (ideal ring). Thus, an algorithm has developed that is close in content to the algorithm in the machine self-learning method (MSL). Modern modeling of nanoscale objects requires a combination of two approaches that were previously developed independently: physically based models of particle interaction and machine learning algorithms. For ring quantum dots and nanorings, such integration is important, since for these objects the structural stability depends not only on the local geometry, but also on collective deformations, the presence of structural defects, and the spectrum of vibrations.

In this work we consider two variants of a nano-ring

of arbitrary atoms) in the XZ plane (Fig. 1), in which the ring is stabilized by “angular springs” and radial anchoring to the circumference, and weak interatomic Lennard-Jones (LJ) interactions [1]. The parameters of an ideal ring (A) and the ring (B) with vacancy are investigated. Specific angular stiffness as the $\rho(\theta)$ distribution is introduced. The effect of vacancy on the anisotropy of the angular stiffness and the character of deformations is investigated. Throughout, the classical molecular-modeling viewpoint is applied to get the stability parameters of the nano-ring ($\theta, \Delta\theta, r_i$) [2].

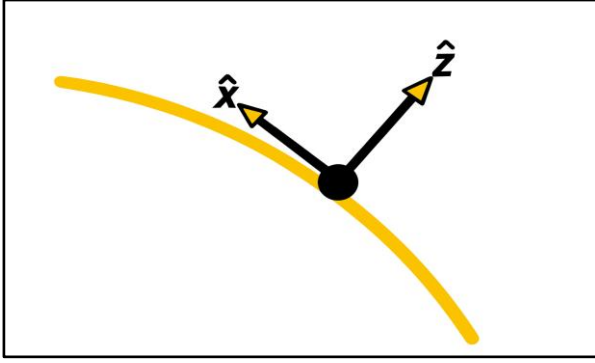


Fig. 1. Fragment of a nano-ring and local base vectors.

I. Notation and Program for Calculation

The program, written in Python, allows one to study the stability of an atomic nano-ring of radius R , in which each atom is connected to the reference circumference by a radial spring with prescribed parameters. For every atom, a reference angle (local angular anchor) and a reference radius are defined. The simulation showed that atoms perform small oscillations around their equilibrium positions. This local behavior is caused by elastic interactions that ensure the stability of the nano-ring in both variants A and B.

The equilibrium angle of atom is θ^0 . The current angles are θ . The equilibrium radius of atom is $r \approx R$. The angular step between neighbors is $\Delta\theta = (\theta_i - \theta)$, the reference step is $\Delta\theta^0 = 2\pi/N$.

All variables and notations are introduced programmatically; the corresponding code listing is given in Appendix 1 [3].

II. Interaction forces

During the research, it turned out that it is advisable to consider the machine self-learning method (MSL) as a basic scheme. In this case, one's own highly reliable intermediate results are iteratively used to obtain the final optimal result.

To build a stable nano-ring structure we are introducing a harmonic force (“radial anchor”) for each atom. The potential energy with minimum at R is:

$$U_r = \frac{1}{2} k_r (r_i - R)^2 \quad (1)$$

Here:

k_r is the radial stiffness coefficient;

r_i is the current distance from the center of the nano-ring

to the i -th atom;

R is the reference (target) radius of the nano-ring.

The restoring force for the radius (Hooke's law) is

$$F_i^{(r)} = -k_r (r_i - R) \hat{r}_i \quad (2)$$

The angular potential energy is:

$$U_\theta^{loc} = \frac{1}{2} k_\theta (\theta_i - \theta_i^0)^2 \quad (3)$$

Here:

k_θ is the angular stiffness of the local “anchor”;

θ_i is the current polar angle of the atom;

θ_i^0 is the reference (equilibrium) angle for the atom.

By analogy to formula (2):

$$F_i^\theta = -k_\theta (\theta_i - \theta_i^0) \quad (4)$$

Thus, according to our approach the equilibrium position of atoms in the nano-ring is determined mainly by two Hooke forces. But it was obtained that to achieve complete stability it's reasonable to add also interactions between neighboring atoms by a weak LJ potential and van der Waals attraction [4]. Because of the significant contribution of elastic forces to the potential of atomic interactions atoms of the nano-ring can under normal conditions perform small vibrations (Fig. 2), which change their profile in the vicinity of a vacancy (Fig. 3).

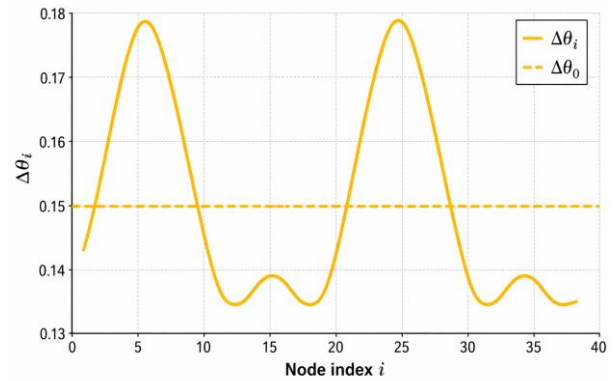


Fig. 2. Profile of $\Delta\theta$ along the ring: variant A.

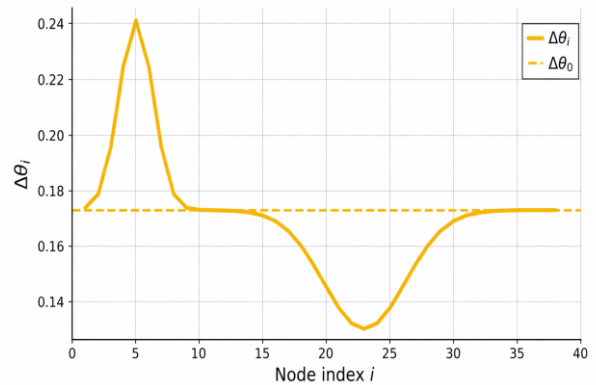


Fig. 3. Profile of $\Delta\theta$ along the ring: variant B.

For variant B it was obtained a “leakage” of neighboring atoms to vacancy. For this variant, after occasional deformation the nano-ring restoration occurs.

In the case of a vacancy (variant B), atoms adjacent to the defect exhibit a characteristic modulation. This effect is shown in Fig. 4.

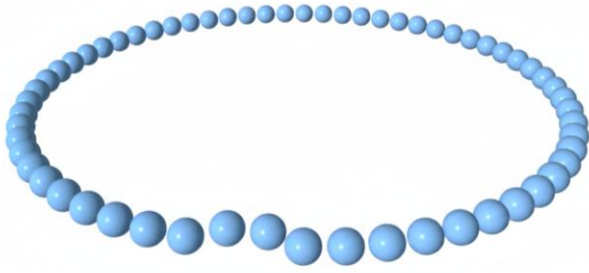


Fig. 4. View of a nano-ring with a vacancy.

It is seen that in the case of variant B, the atoms near the defect exhibit specific behavior.

The comparison of Figures 2 and 3 shows the role of local stiffness in the anisotropy properties connected with defect influence [5].

In the case B (a ring with a vacancy) it was found that small local distortions appear near the defect (Fig. 4).

Using only the LJ potential results in strong distortion of the nano-ring (Fig. 5). Below is shown a perfect nano-ring (Fig. 6).

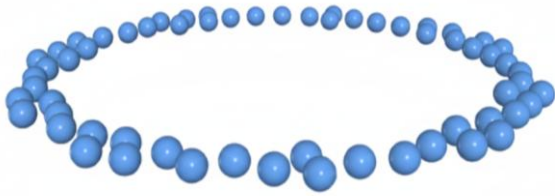


Fig. 5. View of nano-ring obtained with only the LJ potential.

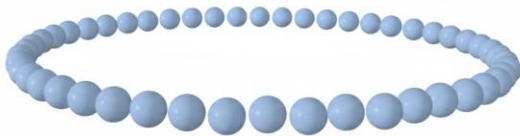


Fig. 6. View of an ideal nano-ring.

In the classical formulation, the MSL does not require a special model structure [6-8]. The basic classifier or regressor can be the support vector method, random forest, gradient boosting, neural network, Bayesian model, or other algorithm capable of making not only a prediction, but also a certain assessment of reliability. It is this versatility that makes the MSL a convenient tool for research in which obtaining a full-fledged marking is expensive or limited by physical experiments.

But in our work, a modification of the MSL is proposed and implemented, namely, a method whose key difference from the MSL is that the “trust criterion” is

improved. The decision to add a pseudo-label is made not only on the basis of the statistical reliability of the result, but also taking into account the compliance with the ideal physical model, the laws of elastic interaction, and the local deformation pattern.

Thus, a modification of the widely known LJ potential has been made for the case when the system has cylindrical symmetry and is located at small distances from the equilibrium position. For these conditions, the LJ potential can be replaced by the N -spring potential. The use of this potential is illustrated for the case of a nanoring. In the case of studying a nanotube, an additional equilibrium equation should be considered.

For a nanoring, it is important to preserve the ring symmetry, the stability of the radius, the value of the interatomic distances and the balance of forces should be consistent with each other. In this case, the problem is reduced to solving two mutually related equilibrium equations (in the radial and tangential directions). To obtain the appropriate solution, a computer program has been developed that provides the solution of the early balance equations with a simultaneous comparison of intermediate results with the standard (ideal ring).

Conclusion

The possibility of constructing a stable nano-ring based on Hooke's radial and angular laws is shown. Essentially, this means that for certain conditions (small deviations of the nanoring atoms from their equilibrium positions), a two-spring potential (2P) is proposed, which is significantly simpler than the LJ potential and allows one to describe the structural features of the nanoring with good accuracy.

Unlike the results obtained with LJ potential, in our case the interaction forces contain a significant dynamic component. It was found that a stable nano-ring is characterized by small radial and angular oscillations (SAO) of atoms. The SAO spectrum has features depending on the defect structure of the nano-ring.

Acknowledgments

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Data Availability Statement: *The original contributions presented in this study are included in the article. Further inquiries can be directed to the corresponding authors.*

Conflicts of Interest: *The authors declare no conflicts of interest.*

Appendix 1:

```
from vpython import *
R, r0 = 0.85, 0.045
scene.width = 800; scene.height = 600
scene.background = color.white
scene.title = "Nano-ring MD (minimal)"
scene.range = R*1.8

N = max(8, int(round(2*pi*R/(2*r0*1.1))))
s = 2*pi*R/N
sigma = s/(2**(1/6.0)); epsilon = 0.012
kR, gamma, dt, vmax = 12.0, 0.05, 0.01, 0.14

def wca(r):
    if r <= 0: return 0.0
    rm = (2**(1/6.0))*sigma
    if r >= rm: return 0.0
    sr = sigma/r; s6 = sr**6; s12 = s6*s6
    return 24*epsilon*(2*s12/r - s6/r)

def radial(p):
    v = vector(p.x,0,p.z); m = mag(v)
    return v/m if m else vector(1,0,0)

pos, vel = [], []
for j in range(N):
    th = j*2*pi/N
    pos.append(vector(R*cos(th), 0, R*sin(th)))
    vel.append(vector((random()-0.5)*0.012, 0,
    (random()-0.5)*0.012))
atoms = [sphere(pos=p, radius=r0, color=color.blue)
for p in pos]

def forces():
    F = [vector(0,0,0) for _ in range(N)]
    for i in range(N):
        F[i] += -gamma*vel[i]
```

```
for i in range(N):
    pi = pos[i]
    for j in range(i+1, N):
        rvec = pi - pos[j]; r = mag(rvec)
        f = wca(r)
        if f == 0: continue
        fij = (f/r)*rvec
        F[i] += fij; F[j] -= fij
    for i in range(N):
        pr = radial(pos[i])
        rmag = mag(vector(pos[i].x,0,pos[i].z))
        F[i] += -kR*(rmag - R)*pr
    return F

while True:
    rate(120)
    a = forces()
    for i in range(N):
        pos[i] += vel[i]*dt + 0.5*a[i]*dt*dt
        pos[i].y = 0
    a2 = forces()
    for i in range(N):
        vel[i] += 0.5*(a[i] + a2[i])*dt
        if vel[i].mag > vmax: vel[i] *= vmax/vel[i].mag
        atoms[i].pos = pos[i]
```

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Структурна стабільність кільцевої квантової точки

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Нанооб'єкти мають широке застосування та активно вивчаються. Вони вирізняються унікальними електронними властивостями. Дослідження їх електронних властивостей неможливе без детальної інформації про їхню атомну структуру. У цій статті представлено підхід, який дозволяє прогнозувати стабільність нанокільця за допомогою класичних наближень. Запропонований підхід використовується для дослідження одношарового нанокільця, яке по суті є квантовою точкою, вирізаною з нанотрубки. Підходи, засновані на методах машинного навчання, в даний час часто використовуються для вирішення подібних задач. Однак класичні наближення не втратили свого значення та виявляються корисними в низці випадків. У цій статті введено силу Гука для кутової та радіальної стабілізації нанокільця. Це дозволяє сформулювати умови структурної стабільності кільцевої квантової точки.

Ключові слова: нанооб'єкти, нанокільце, потенціал Леннарда-Джонса, потенціал двох пружин, сили Гука, локальні коливання, квантова точка.