MODELING THE ADSORPTION PROCESSES AND LUMINESCENCE PROPERTIES OF THE METAL OXIDE ZnO NANOPARTICLES

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Modeling the adsorption processes and luminescence properties of Zinc Oxide (ZnO) can provide valuable insights into its applications. We used Molecular Dynamics (MD) method to investigate the adsorption processes on ZnO nanoclusters under different initial conditions. To ensure the nanoclusters were correctly structured, we applied Radial Distribution Functions (RDF) and Central Symmetry Parameter (CSP) methods. It was discovered that the number of defects in the samples had a major influence on the simulated photoluminescence (PL) spectra, which were created using a bi-Gaussian function. To assess the amount of vacancies on the surfaces of the sample, we used the relative luminescence intensity of the secondary peak in the PL spectra. To analyze the simulated PL spectra, we utilized a Gaussian fitting technique. The self-activated PL band peaking was divided by Gaussian deconvolution, which was utilized for a more in-depth analysis of the data. By researching the consequences of varying conditions on the PL spectra, we were able to obtain a better comprehension of the mechanisms behind adsorption processes on ZnO nanoclusters. Furthermore, this research enabled us to gain insight into the influences that different conditions can have on the adsorption of oxygen atoms on the nanoclusters and helped us in creating new generation gas sensors based on ZnO nanopowders and its compounds.

Key words: molecular dynamics, adsorption, photoluminescence, zinc oxide.

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I. INTRODUCTION

The development of nanotechnologies has generated substantial interest in the exploration of the properties of nanoparticles and their synthesis. Investigating nanoparticles will enable a broad comprehension of the processes of phase transitions and self-organization in complex, dispersed systems. Currently, the study of individual nanoparticles is one of the most swiftly advancing fields of research in physics, chemistry, and engineering. The immense scientific and practical value of such studies is due to the extraordinary properties of nanoparticles, which are already being used or will be utilized in the future for the fabrication of miniature electronic devices and the production of novel materials.

Currently, there is a significant research emphasis on metal oxide nanomaterials due to their distinct physicochemical properties. These nanoparticles are highly beneficial for the fabrication of miniature electronic devices and the production of innovative materials, leading to a great deal of scientific and practical attention. In the crystal structure of Zinc oxide (ZnO), each unit cell comprises one oxygen atom bonded to two distinct zinc atoms. The two zinc atoms are connected to the oxygen atom in an octahedral arrangement, forming a three-dimensional lattice. The lattice structure of ZnO gives it a variety of properties that can be used in chemical and industrial processes. ZnO is an efficient compound for use in electronic devices, solar cells, and gas sensor systems [1–6], due to its high electrical conductivity and low cost.

The most popular way to obtain nanoparticles is to evaporate solid metal in a reactive gas atmosphere. This is known as the gas-phase method [7]. A method for synthesizing metal oxide nanopowder via pulsed laser ablation of a metal target (e.g., Zn, Sn, etc.) in a chemically active environment has been proposed by us [8, 9]. The laser pulse heats the metal pellet to a high temperature, causing atoms to evaporate into the background gas, which assists in reducing the kinetic energy and chemical interaction of the evaporated atoms, resulting in the formation of nanoclusters. When certain conditions are met, near-surface oxidation of nanoparticles occurs during the laser-reactive synthesis process. This process refers to a method of creating nanomaterials, such as metal oxide nanoparticles, by using a high-energy laser pulse to heat a metal target in a chemically active environment, typically a reactive gas. This process causes the metal atoms to evaporate and react with the surrounding gas, leading to the formation of nanoclusters or nanoparticles. These nanoparticles are separated from the target surface in the form of droplets or formed in a vapor-phase burner from metal target atoms, allowing for the creation of complex materials, such as “core-shell” nanopowders [10, 11]. By adjusting the parameters of laser radiation and background gas pressure, the structure, size, and thickness of the oxide layer of the obtained structures may be regulated.

It is well established that the characteristics of nanoparticles are a consequence of their structure, shape, and size, which are the result of their growth [12, 13]. Experimentally investigating the mechanisms of nanoparticle formation is a complex and time-consuming

task, due to the speed of the processes and the minute size of the objects. In the conditions of experimental gas-phase synthesis, the influence of the basic parameters of the synthesis on the physicochemical and structural properties, as well as the external form of the resulting particles, is difficult to study in detail. Therefore, computer simulation is a viable and promising alternative to study the mechanisms of nanostructure formation. Using computer simulation methods, we can study the processes of growth and synthesis of nanoparticles in condensation from the gas phase in detail [14–16]. In this work, we studied the adsorption processes of oxygen atoms on ZnO nanoclusters under different initial conditions using the molecular dynamics method.

Typically, Zinc Oxide (ZnO) displays two distinct types of light emission - one in the ultraviolet spectrum (UV) and another in the visible light spectrum [17, 18]. Nonradiative exciton recombination induces UV emission. However, the mechanism behind the visible PL remains an open problem and is currently widely investigated in terms of defect structure analysis. The green emission, characterized by its high intensity, is the most controversial emission region within the visible spectrum of ZnO [19]. The deconvolution of PL spectra is accomplished through the application of the Gaussian fitting technique. This approach entails fitting a Gaussian curve to the data points within the spectrum, enabling the identification and separation of individual components. The end result is a more precise representation of the spectrum, characterized by heightened clarity and diminished redundancy.

II. MODEL AND METHOD

Molecular Dynamics (MD) method is a powerful technique for simulating adsorption of gas atoms on the surface of ZnO nanoparticles. It provides valuable insights into the adsorption process. This method involves numerically solving Newton's differential equation of motion for every atom in the system, starting from initial values of velocities and coordinates [20–22]. In classical MD, the interaction between atoms is described by empirical force fields that have been parameterized based on spectroscopy studies of small molecules and quantum chemical calculations. These force fields are used to calculate the interatomic potential, which is the primary measure of the strength of interaction between the particles. Particles in classical MD are usually represented as point masses, since the aim is to simulate the system as accurately as possible. To achieve this, the force field must accurately model the physical and chemical properties of the system in question.

The choice of interatomic potential for a given physical experiment is a critical element to consider. In this regard, ReaxFF, a method that combines the results of quantum mechanics and empirical interatomic potential within the formalism of the bond order [23, 24], is typically used to model nanostructures. This potential has been successfully developed for a wide range of chemical compounds, including ZnO, and has already been applied in our previous work on the formation of ZnO nanoparticles in a chemically active environment [25–27]. In these works, simulations of nanoclusters formation processes were carried out, the results of which correlate with the results of this work, in particular the results of using Radial Distribution Functions and Central Symmetry Parameter methods. This technique is based on a molecular dynamics approach, which allows for the calculation of the atomic charges and a detailed description of the atomic positions. Moreover, the potential can be adjusted to account for different physical properties, such as the electrostatic interactions between atoms, and thus can be used to simulate a wide range of materials.

In our mathematical investigations, we systematically varied the initial ZnO cluster sizes, spanning diameters ranging from 2 nanometers to 10 nanometers. Furthermore, we obtained controlled alterations of the oxygen concentration within the system, spanning a range from 10^{17} to 10^{19} atoms per cubic centimeter (atoms/cm^3). These deliberate modifications allowed us to comprehensively explore the structural and compositional effects on our studied phenomena.

In addition, the total energy of the system and the Radial Distribution Functions (RDF) are typically used to describe adsorption processes [21]. The radial distribution function (RDF) enables one to ascertain the probability of two atoms being at a certain distance from each other. The following equation illustrates how the RDF, $g(r)$, is calculated in molecular dynamics simulations:

$$g(r) = \frac{1}{\rho 4\pi r^2 \delta r} \cdot \frac{\sum_{t=1}^{T} \sum_{j=1}^{N} \Delta N(r^{\Delta} \to r + dr)}{N \times T}, \quad (1)$$

where ρ is the concentration in the systems, T is the total simulation time (steps), N is the total number of atoms and r is the radius, the distance from the atom.

Furthermore, we used the Central Symmetry Parameter (CSP) method to study surface properties [28, 29]. We calculated the CSP for the near-surface layers of nanoclusters using the formula:

$$\mathrm{CSP} = \sum_{i=1}^{N/2} |\mathbf{R}_i + \mathbf{R}_{i+N/2}|^2, \quad (2)$$

where N are the nearest neighboring atoms of the i-th atom, $\mathbf{R}_i$ and $\mathbf{R}_{i+N/2}$ are vectors from the central atom to a specific pair of nearest neighbors. In solid state systems, CSP is a useful characteristic of the local arrangement of the lattice around the atom. It can be used to determine if an atom is part of an ideal lattice, a local defect, or on the surface. For a cubic face-centered lattice, a CSP value of 0 means the atom is surrounded by neighboring atoms on an ideal lattice. The CSP value of 0 indicates that the atom in question is perfectly surrounded by neighboring atoms arranged in an ideal lattice. In other words, it suggests that the local atomic environment is in a highly ordered and regular crystal

structure. The larger the value of the central symmetry parameter, the more the structure deviates from the ideal one. By studying the CSP values of different nanocluster surfaces, we can gain a better understanding of the properties of the surface and the interactions between the atoms.

To study PL properties, we have simulated PL spectra for ZnO. Generally, PL spectra of a substance have several emission bands, some of which are intrinsic and others caused by defects. To generate simulated PL data, the emission band wavelengths, relative strengths and widths must be described. Peaks are often asymmetric when plotted as a function of wavelength or energy, due to factors such as phonon replicas and band-tail states. In this work, we use a bi-Gaussian function to empirically describe each emission peak:

$$I = \begin{cases} A\exp\left(-\frac{(x-x_0)^2}{2\sigma_1^2}\right), & x < x_0, \\ A\exp\left(-\frac{(x-x_0)^2}{2\sigma_2^2}\right), & x > x_0, \end{cases} \tag{3}$$

where A is the relative peak height, x_0 is the peak center position, variable x corresponds to $h\nu$, σ_1 and σ_2 are the left and right standard deviations that describe the asymmetric width of the peak. We restricted the data to PL spectra collected at room temperature. For ZnO, there is usually a UV peak at 378 nm due to free-exciton recombination and a broad green band near 530 nm due to defects [30].

The complex PL band spectra may be due to multiple components and can typically be deconvoluted into individual components. The spectrum is deconvoluted based on the process governing each component. Generally, the luminescence process is described by a Gaussian line broadening mechanism. In this case, the luminescence intensity can be expressed as a Gaussian line-shape function, as expressed by the following equation:

$$I(h\nu) = I_0 + \sum_{i=1}^{N} A_i \exp\left(-\frac{h\nu - E_{0i}}{2\sigma_i^2}\right), \tag{4}$$

where $h\nu$ is the energy of the radiation emitted, I_0 is the offset intensity, A_i is the amplitude of each component, E_{0i} is the energy of each component in which the intensity is maximum, and σ_i is the standard derivation for each component [31].

III. RESULTS AND DISCUSSION

To investigate the mechanism of oxygen molecule adsorption on the ZnO nanocluster surface, a series of computer simulations were carried out using molecular dynamics. At high temperatures, small nanoclusters began to melt quickly, making it difficult to trace the evolution of the system. When larger nanoclusters were selected, the modeling times became too long. Thus, it was necessary to select the optimal initial conditions. The main parameters of the control system were implemented to ensure the accuracy of the experiment from a physical perspective. Temperature control was achieved through the release of energy during oxidation of the nanocluster surface. In real-world scenarios, this control is provided with reactive gas, but in our case, we introduced the concept of a thermostat to remove excess heat. Figure 1 illustrates a nanocluster at the start of the simulation.

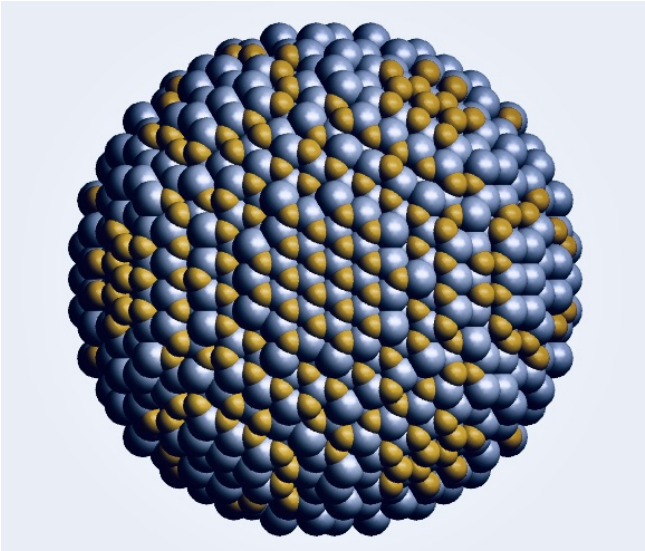

Fig. 1. Snapshot of the ZnO nanocluster at the initial moment of the simulation

At room temperature (300 K), the thermal oscillations of nanocluster atoms can be disregarded if we are mainly interested in the interaction with the absorbed molecule, rather than the physical behavior of the crystal itself. We added oxygen atoms to the system and observed the main parameters. We tracked changes over time, choosing a 5 fs step in the adsorption models for a more detailed observation of the structural evolution process.

The peaks of the RDF curves (Fig. 2), which are indicative of the interatomic distances between atoms, correspond to the distance between the two atoms. Initially, the most prominent peak is observed near 2 Å, which is characteristic of O–Zn pairs. As the concentration of O atoms in the system increases, the peak increases in size, indicating that there is an increase in the number of O–Zn pairs. This is a strong indication of the formation of stable O–Zn bonds, which is crucial for the proper functioning of the system. Furthermore, the growth of the peak also indicates that the interactions between the O and Zn atoms are becoming more and more significant, thus leading to more effective interactions between the two atoms.

Our research indicates that adsorption occurs in two distinct stages. First, a rapid increase in the number of adsorbed atoms is observed, followed by more pronounced fluctuations in their concentration over time. Furthermore, we have established a correlation between the gas pressure in the system and the diffusion rate of oxygen atoms into the ZnO nanocluster. As the gas pressure increases, more oxygen atoms can diffuse

into the nanocluster, leading to a transformation in the crystal structure of its surface to an amorphous form. This finding highlights the importance of gas pressure for the adsorption process of ZnO nanoclusters and points to a potential mechanism for controlling the adsorption rate.

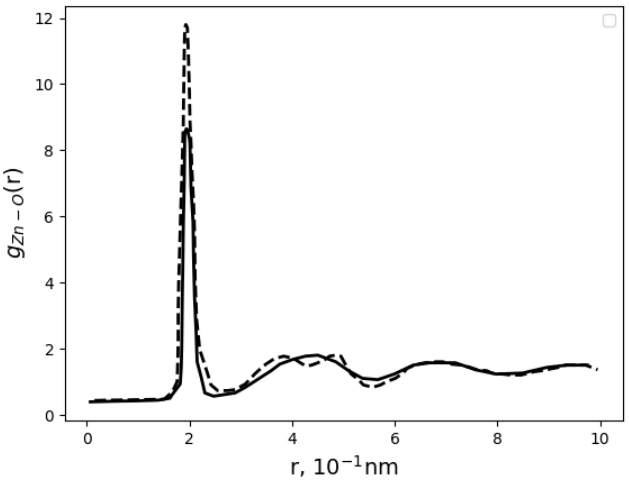

Fig. 2. Radial distribution functions of ZnO nanoparticle for O–Zn pairs at the initial moment of the simulation (line), end of simulation (dashed line)

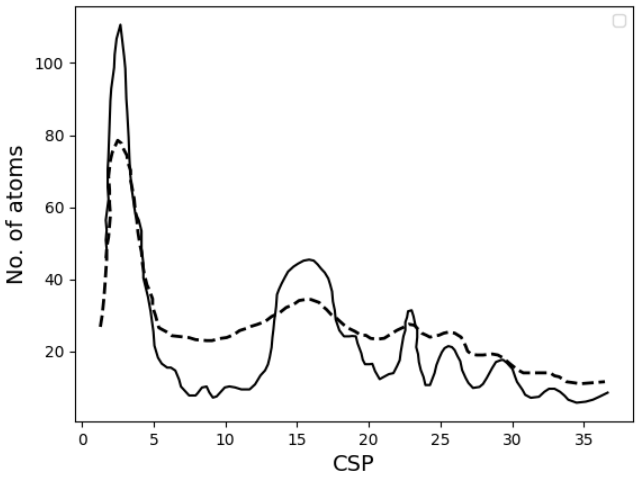

Fig. 3. Central Symmetry Parameter analysis of the surface sublayer of the ZnO nanocluster at the initial moment of the simulation (line), end of simulation (dashed line)

Figure 3 presents the outcomes of CSP calculations, showing that for systems with less than 500 atoms, the tendency of the parameter's dependence on the oxygen concentration is alike: all of them having a significant peak in the interval of 4 Å, indicating that they still maintain a relatively crystalline structure on the surface. However, when the oxygen atoms count elevates, the central symmetry parameter of surface atoms experiences a more even distribution, and the peaks become less discernible. The central symmetry parameter of surface atoms displayed a more uniform distribution, characterized by a single prominent peak, indicating a departure from a crystalline state in the ZnO nanoparticle. This analysis confirms our initial hypothesis, providing more concrete evidence that the structure of the surface is affected by the number of oxygen atoms present. Understanding the connection between the two, it is possible to optimize the surface structure for desired outcomes.

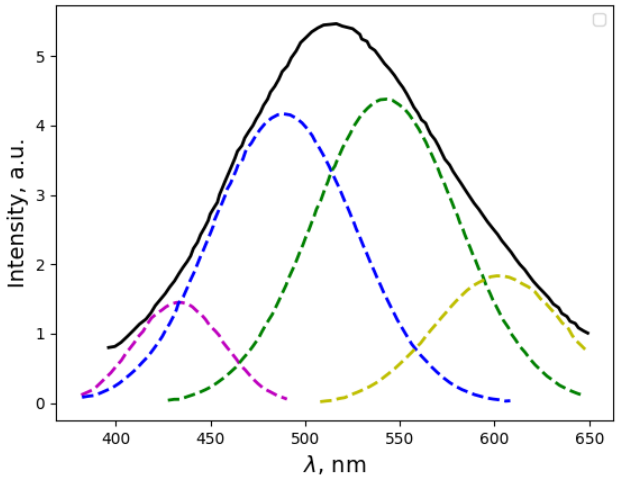

Fig. 4. Deconvoluted photoluminescence spectra of ZnO nanostructures at the initial moment of the simulation

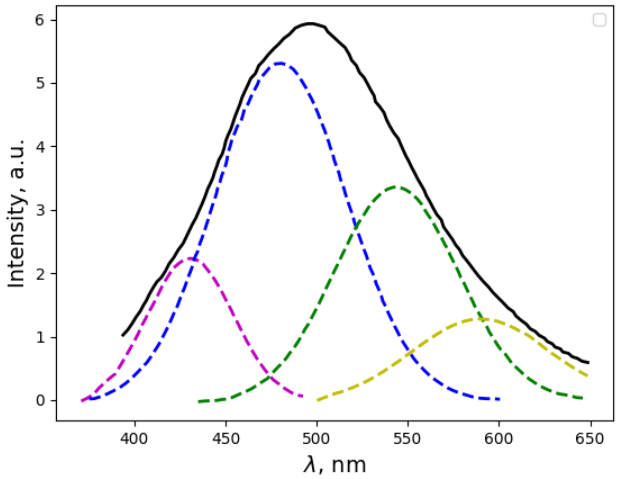

Fig. 5. Deconvoluted photoluminescence spectra of ZnO nanostructures at the final moment of the simulation

In this section, we will provide detailed examples of deconvolution analysis for generated PL curves for ZnO nanclusters. To achieve at a more thorough understand-

ing of the data, we will be utilizing the Gaussian fitting technique in a Python computing environment. This technique is effective in providing a more comprehensive view of the data, as it can generate a more accurate representation of the PL curves. We will be using this approach in order to gain a deeper insight into the data, and to obtain more precise results.

Figure 4 shows generated PL spectra for ZnO with deconvoluted curves at the initial moment of the simulation. It is evident that there are four PL components, which represent different types of electronic transition and are linked to a specific structural arrangement. The violet (violet dashed line) and blue (blue dashed line) emissions are attributed to the transition from $I_{\mathrm{Zn}}(I_{\mathrm{Zn}} \mapsto VB)$ and extended I_{Zn} states (ex-$I_{\mathrm{Zn}} \mapsto V_{\mathrm{Zn}}$) to the valance band, respectively [32–34]. The green emission is the most dominant peak, and it comprises two components: $V_{\mathrm{O}}^{*} \mapsto VB$ (green dashed line) and $CB \mapsto V_{\mathrm{O}}^{++}$ (yellow dashed line). All these cases demonstrate correctness in the peak intensity of $V_{\mathrm{O}}^{*} \mapsto VB$ compared to (ex-$I_{\mathrm{Zn}} \mapsto V_{\mathrm{Zn}}$). However, the peak intensity of $CB \mapsto V_{\mathrm{O}}^{++}$ is found to be lower than $V_{\mathrm{O}}^{*} \mapsto VB$ in all cases.

Increasing the gas pressure (Fig. 5) results in a greater intensity of violet and blue emissions. Notably, in the case of ZnO nanoparticles, the emission from (ex-$I_{\mathrm{Zn}} \mapsto V_{\mathrm{Zn}}$) is more pronounced than the emission from $V_{\mathrm{O}}^{*} \mapsto VB$. Furthermore, the peak at $\sim$ 465 nm corresponds to the blue emission, which shifts to 480 nm when the concentration of O atoms in the system is increased. This is an important observation, as it suggests that the concentration of O atoms has a direct influence on the emission intensity of the blue wavelength. Furthermore, this implies that the higher the concentration of O atoms, the higher the intensity of the blue emission.

IV. CONCLUSIONS

We used molecular dynamics to model the adsorption of O atoms on ZnO nanoclusters under various initial conditions. It was established that as the concentration of O atoms increased, the peak of the RDF curves rose considerably, indicating a heightened amount of O–Zn pairings. This indicates that, when the concentration of O atoms is high, the chances of creating O–Zn pairings are significantly higher compared to other concentrations. Furthermore, the distribution of the central symmetry parameter's dependence on oxygen concentration was similar in the system with less than 500 oxygen atoms. All of them had a pronounced peak in the range of 4 Å, indicating that they still maintained a relatively crystalline structure on their surface. When the number of oxygen atoms increased, the situation changed drastically. The central symmetry parameter of surface atoms was more evenly distributed, and there was one clear peak, indicating that the ZnO nanoparticle was not in a crystalline state. We carried out a detailed deconvolution analysis of the generated PL curves using the Gaussian fitting technique. This revealed four peaks, each corresponding to a different type of electronic transition. The gas pressure increased, resulting in an increase in the violet and blue peaks. This is significant, as it implies that the concentration of O atoms has a direct effect on the intensity of the blue wavelength emission.

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МОДЕЛЮВАННЯ ПРОЦЕСІВ АДСОРБЦІЇ ТА ЛЮМІНЕСЦЕНТНІ ВЛАСТИВОСТІ МЕТАЛООКСИДНИХ НАНОЧАСТИНОК ZnO

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Моделювання адсорбції та властивостей люмінесценції оксиду цинку (ZnO) може дати цінну інформацію про його застосування. У цьому дослідженні ми використовували метод молекулярної динаміки (МД) для вивчення адсорбції на нанокластерах ZnO за різних початкових умов. Для того щоб забезпечити правильну структуру нанокластерів, ми застосували методи радіальних функцій розподілу (RDF) і центрального параметра симетрії (CSP). Виявлено, що кількість дефектів у зразках мала великий вплив на модельовані спектри фотолюмінесценції (ФЛ), які були створені за допомогою функції Ґаусса. Для оцінки кількості вакансій на поверхні нанокластера використовували відносну інтенсивність люмінесценції вторинного піка в спектрах ФЛ. Для аналізу змодельованих спектрів ФЛ ми застосували методику підгонки Ґаусса. Пікове значення самоактивованої смуги ФЛ поділили деконволюцією Ґаусса, яка була використана для глибшого аналізу даних. Досліджуючи вплив різних умов на спектри ФЛ, ми змогли ліпше зрозуміти механізми адсорбції на нанокластерах ZnO. Крім того, це дослідження дало змогу отримати уявлення про вплив різних умов на адсорбцію атомів кисню на нанокластерах і допомогло нам в розробці сенсора газу нового покоління на основі нанопорошків ZnO та його сполук.

Ключові слова: молекулярна динаміка, адсорбція, фотолюмінесценція, оксид цинку.