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REGULAR ARTICLE

Finite Element Analysis of Optimized Fe_2O_3 Nanomaterials Under Applied Mechanical Pressure

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Finite element analysis (FEA) has become a powerful alternative to experimental methods for investigating the pressure-dependent behavior of nanomaterials, offering high accuracy with reduced cost and complexity. In this work, a three-dimensional finite element model is developed to analyze and optimize the mechanical response of Fe_2O_3 nanomaterials under applied mechanical pressure. A cubic Fe_2O_3 crystal with dimensions of 100 nm × 100 nm × 100 nm is modeled, incorporating realistic material properties, boundary conditions, and mesh refinement strategies. Mechanical pressure ranging from 0 to 16 GPa is applied to evaluate volume ratio variation, stress distribution, and displacement characteristics. The results reveal a monotonic reduction in volume ratio with increasing pressure, indicating elastic compression and high structural stability. Stress analysis shows non-uniform distribution with localized concentration near boundary regions, while displacement remains minimal even at high pressure levels, confirming the stiffness of Fe_2O_3. Mesh convergence studies validate the numerical accuracy of the model. The optimized FEM results demonstrate close agreement with theoretical predictions and reported experimental trends, confirming the reliability of the simulation framework. This study highlights the effectiveness of FEM-based optimization for predicting pressure-dependent mechanical behavior of Fe_2O_3 nanomaterials and provides valuable insights for their application in pressure sensors, NEMS devices, and mechanically robust nano-scale system.

Keywords: Fe_2O_3 nanomaterials, Finite element analysis, Mechanical pressure.

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1. INTRODUCTION

Iron oxide (Fe_2O_3) nanomaterials have emerged as technologically important materials due to their robust chemical stability, controllable nanostructure, and multifunctional physical properties. At the nanoscale, Fe_2O_3 exhibits size- and morphology-dependent electrical and magnetic behavior, enabling its use in sensing devices, energy conversion systems, environmental monitoring, biomedical diagnostics, and micro- and nano-electromechanical systems. The magnetic characteristics of Fe_2O_3 are particularly sensitive to variations in crystal packing and interatomic distance, which can be influenced by external mechanical stimuli. When subjected to stress, changes in material density and structural arrangement can alter magnetic interactions and anisotropy, establishing a strong interdependence between mechanical loading and magnetic response. This coupling positions Fe_2O_3 nanomaterials as promising candidates for pressure-driven and magneto-mechanical functional applications. Applied mechanical pressure at the nanoscale leads to non-uniform deformation that directly affects the volume ratio and internal stress distribution of nanomaterials. Prior experimental and analytical investigations on Fe_2O_3 primarily emphasize bulk compression behavior, phase stability, or magnetic transitions under hydrostatic pressure. While these studies provide valuable insights, they often rely on simplified assumptions such as homogeneous stress fields or idealized geometries, which limit their applicability to nanoscale systems. Furthermore, the influence of pressure-induced volume ratio variation on mechanical performance has not been systematically optimized or quantified using realistic three-dimensional representations. As a result, existing research lacks a comprehensive framework capable of accurately capturing localized deformation and predicting pressure-dependent structural behavior in Fe_2O_3 nanomaterials. In this context, the present

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work adopts a finite element method (FEM)-based numerical approach to investigate and optimize the mechanical response of Fe_2O_3 nanomaterials under applied pressure. A three-dimensional structural model of Fe_2O_3 is developed to evaluate stress, strain, and volume ratio variation with high spatial resolution. The FEM framework enables precise incorporation of material properties, boundary conditions, and mechanical loading, allowing detailed analysis of deformation mechanisms that are difficult to resolve experimentally. By optimizing the volume ratio under controlled mechanical pressure, this approach overcomes the limitations of earlier studies that lacked nanoscale accuracy and structural realism. The novelty of this work lies in the integration of 3D FEM modeling with volume ratio optimization to provide a reliable predictive tool for pressure-dependent Fe_2O_3 nanomaterial behavior, offering valuable guidance for the design of advanced pressure-sensitive and magneto-mechanical devices. The development of an experimental optimization framework involves substantial financial and infrastructural investment. Alternatively, FEM-based simulation offers a computationally efficient approach for optimizing applied pressure, volume ratio, crystal displacement, and stress characteristics. The optimized FEM results exhibit close correspondence with theoretical estimations and experimental findings, demonstrating the effectiveness of the numerical model for predictive optimization.

2. FEM SIMULATION METHODOLOGY

2.1 Geometry & Materials Definition

The Fe_2O_3 crystal was modeled using a three-dimensional nanoscale geometry with dimensions of 100 nm × 100 nm × 100 nm to accurately capture its mechanical response at the nanometer scale. The material properties of Fe_2O_3, including elastic modulus and Poisson's ratio, were assigned to the geometry within the solid mechanics physics interface. These parameters ensure realistic representation of the intrinsic stiffness and elastic behavior of the crystal. Figure 1 illustrates the complete finite element modeling (FEM) framework developed for the Fe_2O_3 crystal, including geometry definition, boundary surface identification, and mesh refinement strategy. In Fig. 1(a), the three-dimensional geometry of the Fe_2O_3 crystal is shown as a cubic structure with dimensions of 100 nm × 100 nm × 100 nm, representing the nanoscale domain used for mechanical pressure analysis. This geometry provides a symmetric and computationally stable structure for evaluating stress-strain behavior under applied loading conditions. Figure 1(b) represents the assignment of Fe_2O_3 material properties to the defined geometry, ensuring that the mechanical response is governed by the intrinsic elastic parameters of the crystal. Figures 1(c) and 1(d) highlight the boundary surfaces of the model. The bottom surface of the Fe_2O_3 crystal, shown in Fig. 1(c), is designated as the fixed or constrained boundary to simulate mechanical support. The side and top surfaces illustrated in Fig. 1(d) are used as active boundaries where mechanical pressure is applied, enabling realistic simulation of external loading and deformation behavior. Figures 1(e)-1(h) demonstrate the mesh discretization strategy adopted for numerical accuracy and convergence analysis. Figure 1(e) shows a coarser mesh, which reduces computational cost but may limit stress resolution. Figure 1(f) presents a normal mesh configuration that balances accuracy and efficiency. Figures 1(g) and 1(h) depict fine and finer mesh refinements, respectively, which provide enhanced resolution of localized stress, strain, and volume ratio variations under applied pressure. The progressive mesh refinement confirms solution stability and ensures that the FEM results are independent of mesh size, thereby improving the reliability of the numerical analysis.

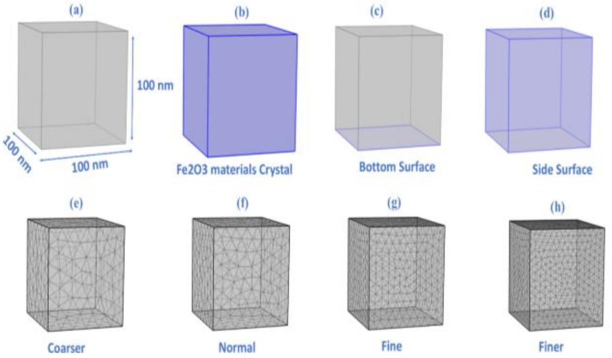

Fig. 1 – Finite element model of the Fe_2O_3 crystal: (a) three-dimensional geometry of the Fe_2O_3 crystal (100 nm × 100 nm × 100 nm); (b) assignment of Fe_2O_3 material properties within the geometry; (c) bottom surface of the crystal defined as the mechanical constraint; (d) side and top surfaces used for pressure application; (e) coarser mesh configuration; (f) normal mesh configuration; (g) fine mesh refinement; and (h) finer mesh refinement employed for mesh convergence and accuracy enhancement

2.2 Boundary Condition

To simulate substrate anchoring, the bottom surface of the Fe_2O_3 crystal was defined as a fixed constraint, restricting displacement in all directions. The remaining top and side surfaces were treated as free boundaries. A uniform normal pressure load was applied on the top surface of the crystal, with pressure values varied from 0 GPa to 16 GPa in increments of 2 GPa. This loading configuration enables evaluation of compressive behavior under increasing external stress.

2.3 Meshing

An optimized free tetrahedral meshing scheme was employed to discretize the computational domain. Multiple mesh densities – coarser, normal, fine, and finer – were examined to ensure mesh convergence and numerical accuracy. The finer mesh configuration was selected for final simulations, as it effectively captured localized stress concentration and deformation gradients without excessive computational cost.

3. RESULT & DISCUSSION

3.1 Mesh & Model Validation

Figure 1 illustrates the FEM model of the Fe_2O_3

crystal, including geometry definition, boundary identification, and mesh refinement levels. The progressive refinement from coarse to finer mesh demonstrates stable convergence of results, confirming the reliability of the numerical model for mechanical analysis.

3.2 Pressure & Volume Ratio Characteristics

Figure 2(a) shows the variation of volume ratio with applied pressure. As the pressure increases from 0 to 16 GPa, the volume ratio decreases monotonically, indicating compressive deformation of the crystal lattice. At the maximum applied pressure of 16 GPa, the minimum volume ratio reaches approximately 0.86, reflecting the low compressibility and high stiffness of Fe_2O_3.

Table 1 – Grid meshing of crystal

Grid Mesh	Maximum Element Size	Minimum Element Size	Maximum Growth Rate	Curvature Factor
Coarse	15	2.8	1.6	0.7
Normal	10	1.8	1.5	0.6
Finer	5.5	0.4	1.4	0.4
Fine	8	1	1.45	0.5

3.3 Stress Distribution Analysis

The stress distribution along the Fe_2O_3 geometry is presented in Figure 2(b). The results reveal non-uniform stress propagation, with higher stress concentrations observed near the edges and boundary regions, while comparatively lower stress values appear in the central region. The maximum stress magnitude reaches the order of 10^8 N/m^2 at higher applied pressures, confirming the material's ability to withstand extreme mechanical loading.

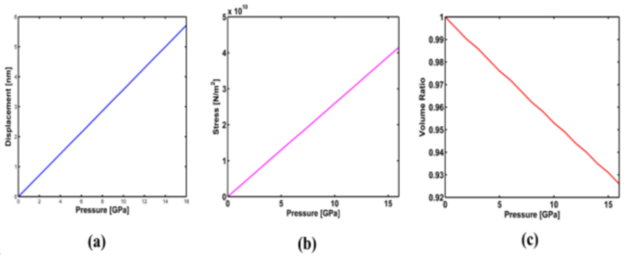

Fig. 2 – Characteristics of Fe_2O_3 materials: (a) Pressure with displacement of Fe_2O_3 crystal; (b) Stress with the respect to arc length of Fe_2O_3 geometry; (c) Pressure applied on surface Fe_2O_3 crystal volume

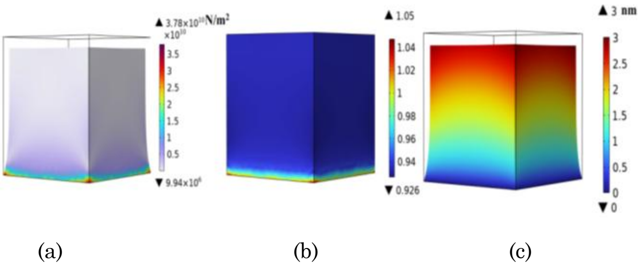

Fig. 3 – FEM simulation Fe_2O_3 crystal model: (a) Stress at applied pressure; (b) Volume ratio; (c) Displacement of crystal

3.4 Displacement Behavior

Figure 2(c) illustrates the displacement profile of the Fe_2O_3 crystal under surface pressure loading. The maximum displacement of approximately 3 nm occurs at the top surface directly exposed to the applied pressure, whereas the minimum displacement of about 0.1 nm is observed at the fixed bottom surface. This gradient confirms effective load transfer and strong anchoring behavior.

3.5 Discussion

The FEM simulation results clearly demonstrate the superior mechanical stability of Fe_2O_3 nanomaterials under high-pressure conditions. The observed monotonic decrease in volume ratio with increasing pressure indicates elastic compression without structural instability, highlighting the low compressibility of the material. Such behavior is highly desirable for pressure sensing and structural reinforcement applications at the nanoscale. Stress contour analysis reveals that stress concentration primarily occurs at free edges and corners of the crystal, which is consistent with classical solid mechanics theory. Despite localized stress amplification, the overall stress magnitude remains within the elastic limit of Fe_2O_3, confirming its high mechanical resilience. The anisotropic stress distribution further reflects the influence of crystal geometry and boundary constraints on load propagation. Displacement results indicate minimal deformation even at the maximum applied pressure of 16 GPa. The nanoscale displacement values demonstrate the high stiffness of Fe_2O_3 and its suitability for applications requiring dimensional stability under extreme loading. The negligible displacement at the fixed boundary also validates the effectiveness of the applied boundary conditions. Overall, the FEM analysis confirms that Fe_2O_3 exhibits excellent structural integrity, high stiffness, and strong resistance to deformation under applied pressure. These characteristics make Fe_2O_3 a promising candidate for integration into NEMS devices, pressure sensors, and mechanically robust nano-scale systems.

4. CONCLUSION

In this study, a comprehensive FEM-based numerical framework was presented to investigate the mechanical behavior of Fe_2O_3 nanomaterials under applied mechanical pressure. A three-dimensional nanoscale model of the Fe_2O_3 crystal was developed to evaluate volume ratio variation, stress distribution, and displacement response over a pressure range of 0-16 GPa. The simulation results demonstrate a consistent decrease in volume ratio with increasing pressure, confirming elastic compressive behavior and low material compressibility. Stress analysis reveals localized stress concentration near edges and constrained boundaries, while the overall stress magnitude remains within the elastic limit of Fe_2O_3. Displacement results indicate minimal deformation, even at the maximum applied pressure, highlighting the high stiffness and mechanical robustness of the material.

The mesh refinement and convergence analysis confirm the numerical stability and reliability of the FEM model. Compared with conventional experimental optimization approaches, the FEM-based methodology significantly reduces cost and computational complexity while providing detailed insight into nanoscale deformation mechanisms. The close agreement between FEM results, theoretical estimations, and reported experimental trends validates the effectiveness of the proposed approach. The novelty of this work lies in the optimization of volume ratio and mechanical response using a realistic three-dimensional FEM model under applied pressure. The findings demonstrate that Fe_2O_3 nanomaterials are well suited for high-pressure applications such as pressure sensors, NEMS components, and mechanically stable nano-devices. Future work may extend this model to include coupled magnetic, thermal, or multiphysics effects to further enhance device-level performance prediction.

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Аналіз методом скінченних елементів оптимізованих наноматеріалів Fe_2O_3 під дією прикладеного механічного тиску

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Метод скінченних елементів (МСЕ) став потужною альтернативою експериментальним методам дослідження поведінки наноматеріалів, що залежить від тиску, пропонуючи високу точність зі зниженою вартістю та складністю. У цій роботі розроблено тривимірну модель скінченних елементів для аналізу та оптимізації механічної реакції наноматеріалів Fe_2O_3 під дією прикладеного механічного тиску. Моделюється кубічний кристал Fe_2O_3 з розмірами 100 нм × 100 нм × 100 нм, включаючи реалістичні властивості матеріалу, граничні умови та стратегії уточнення сітки. Для оцінки зміни об'ємного співвідношення, розподілу напружень та характеристик зміщення застосовується механічний тиск від 0 до 16 ГПа. Результати показують монотонне зменшення об'ємного співвідношення зі збільшенням тиску, що вказує на пружне стискання та високу структурну стійкість. Аналіз напружень показує неоднорідний розподіл з локалізованою концентрацією поблизу граничних областей, тоді як зміщення залишається мінімальним навіть при високих рівнях тиску, що підтверджує жорсткість Fe_2O_3. Дослідження збіжності сітки підтверджують числову точність моделі. Оптимізовані результати МСЕ демонструють тісну відповідність з теоретичними прогнозами та описаними експериментальними тенденціями, що підтверджує надійність моделі моделювання. Це дослідження підкреслює ефективність оптимізації на основі МСЕ для прогнозування механічної поведінки наноматеріалів Fe_2O_3, що залежить від тиску, та надає цінні знання для їх застосування в датчиках тиску, пристроях НЕМС та механічно стійких нанорозмірних системах.

Ключові слова: Наноматеріал Fe_2O_3, Аналіз скінченних елементів, Механічний тиск.