Modeling and simulation of mechanical and physical properties of Barium orthotitanate (Ba_2TiO_4) composite by Materials Studio (MS)

Najat A. Dahham[1] , Abdullah Hamoud Fares[2] , Khaled Abdullah Najem[1]
[1]*Department of Physics, College of Science, University of Tikrit , Tikrit , Iraq*
[2] *Department of Physics, College of Education for Pure Sciences, University of Kirkuk , Kirkuk M Iraq*
E-mail: najat_200570@yahoo.com
E-mail :Khalid.you9876@gmail.com

Abstract
This research including a study of mechanical ,physical properties (band structure, density of states) and the elasticity constants of the Barium Ortho titanate by using Materials studio software. The calculations were based on the generalized gradient approximation (GGA) by linear method. The calculated equilibrium lattice constants of monoclinic barium orthotitanate were: a = 0.612nm, b = 0.77nm, c = 1.05nm,calculated bulk modulus =42.3021 GPa, young modulus= 40.29 GPa, share modulus = 15.97 GPa, lame constant (λ)= 142.56 GPa ,and energy band gap=3.435eV which is indirect band gap and the composite is insulator and the electronic properties where be calculated in first Brillion zone. According the mechanical stability conditions the composite is stable mechanically. These results were calculated by Materials studio software.

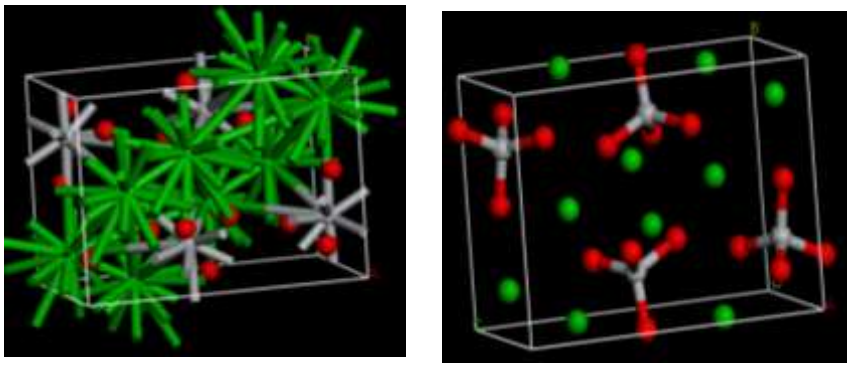
Key words: Molecular dynamic, Geometry optimization, Modeling, simulation.

1. Introduction
As our requirements for materials have increased recently, we focus our attention on how to improve material properties and make them suitable in all aspects of life and in many applications and approaches of mechanical and electronic properties of ceramics to improve its advantages as it received a lot of attention from researchers. Simulation of molecular dynamics is a very important process and an important means of predicting the crystal structure, mechanical properties of ceramic materials. Rooksby study crystal structure in 1947, In 2001, Shackelford studied mechanical properties and mechanical behavior of ceramic and glass materials when exposed to external forces, including ceramics Ba_2TiO_4 and Ding Ying et al study mechanical properties in 2012 and The Materials Simulation Program in Materials Science named Materials Studio, deVeloped by the American Accelrays Foundation is being used extensively in the pharmaceutical, petrochemical, automotive and industries as well as being used by researchers in materials science[1]. Barium ortho titanate Ba_2TiO_4 is a good material for some applications and plays an important role in the scientific researches of composites, Ba_2Tio_4 was first examined crystallographically by Rooksby (1947) who showed that its X-ray powder pattern resembles that of Ba_2Sio_4 which has β-K2So4 structure and have peroviskite crystal structure in two modifications as Rooksby et al and Net rer et al dicoverd[2].

2. Computational Methods
the commercial software package Material Studio, includingthe Cambridge Serial Total Energy Package CASTEP module was used to conduct these simulations the calculationswere performed on a parallel computer cluster consisting of 14 AMD Opteron 64-bit processors utilizing a LINUX based operating system. Starting with the base structure ,a geometric optimization was performed to determine the initial lattice parameters and density[3]. In our calculations, we used the generalized theory of grading(GGA) along with ultra-soft pseudo potentials to represent the atoms. Specifically, for this geometric optimization, the Perdew-Burke-Ernzerhof potential for solids (PBEsol) was used .To obtain accurate band structures, calculations using the GGA PBEsol, as well as the hybrid functional Becke, three parameter, Lee Yang-Parr (B3LYP) potentials, were used. The finite element displacement method applied to a super cell of the geometrically optimized primitive lattice using norm-conserving potentials to calculate the phonon dispersion curves was used. The real space cutoff radius was set to 5 Å which resulted in a super cell volume 493.08 Å³ for Ba_2TiO_4[4].

3. Results
3.1.The crystal structure
Ba_2Tio_4 is found in nature in two forms of monoclinic and orthorhombic crystalline structure[2], the orthorhombic shape cannot be found in stable state except at high temperatures while the other type is stable at normal temperature at room temperatures. The orthorhombic type of Ba_2TiO_4 is troubled compound especially if we are exposure it to air . As Rooksby (1947) found the monoclinic of Ba_2Tio_4 has a β-Ca2So4 structures type and has lattice parameters: a = 0.612nm, b = 0.77nm, c = 1.05nm, α = γ = 90°, β = 92.99°,and the orthorhombic of Ba_2TiO_4 has a β-K2So4 structure and the following lattice parameters: a = 0.765nm, b = 1.055nm, c = 0.61nm, ,(space group is p_{nam}),were this results is agreed with researches [2][5] .Orthorhombic consists of cations of the same compound with quadruple equivalents in a tetrahedral format that is unprecedented from other compounds. The crystal structure is shown in Figure(1),present calculations of lattice constants and experimental values are shown in the table1s hown below[5].

ISSN: 1813 – 1662 (Print)
E-ISSN: 2415 – 1726 (On Line)



(a) **(b)**

Figure.1 shows the crystal structure of Ba_2TiO_4 indifferent forms where (a) is the unit cell and (b) is the primitive cell[6]

Table1 shows Comparison of the theoretical results obtained from the MS program with experimental results[7] for preVious studies showing a good agreement in the results obtained with preVious studies.

Table.1. lattice parameters of the primitive cell

		Simulations
Parameters		
	Present Study (theory)	**Experimental [7]**
a (Å) =	**6.096**	**6.098**
b (Å) =	**7.681**	**7.682**
c (Å) =	**10.545**	**10.544**
α = γ (degrees) =	**90**	**90**
β (degrees) =	**92.990**	**92.990**
Volume ($Å^3$) =	**493.08**	**493.1**
Density (g/cm^3) =	**5.207**	**5.206**

3.2. Simulation steps of mechanical and electronic properties

1.To determine the composite select: File: Import: Structures: Ceramics, and choose the compound Ba_2TiO_4.

2.To build the primitive unit cell choose: Build, Symmetry , Primitive cell, from the menu bar.

3.Geometry optimization, select: Modulus , Forcite , Calculation, and select , geometry optimization from the task dropdown.

4.To calculate mechanical properties select, Modulus, Forcite, Calculation and choose, Mechanical properties from the calculation menu.

5.To calculate electronic properties(density of states and band structure E_g), select: Castep bottom from modulus tool bar and select :Analysis , Density of states or choose ;Band structure, and click Import[8].

3.3.Mechanical properties

The mechanical properties of Ba_2TiO_4 include the elastic constants of the crystalline

and these constants are the result of the response to external forces. There are six components of tensile strength, as well as six other stress-related compounds in the three dimensions 3D of the crystal. Hook's law of elasticity can be expressed on the expression formula[9]:

$\sigma_i = C_{ij}\,\varepsilon_j$ ……..(1)

$\varepsilon_i = S_{ij}\,\sigma_j$……..(2) ,where i,j=1,2,3

Where C = elasticity constant, S = mutant, σ = stress and ε = strain. Hook's low for elasticity that possesses (6×6) compounds on the surface of the material,it can be expressed as in the following formula[10]:

$$\begin{pmatrix}\sigma1\\ \sigma2\\ \sigma3\\ \sigma4\\ \sigma5\\ \sigma6\end{pmatrix} = \begin{pmatrix}C11 & C12 & C13 & C14 & C15 & C16\\ C21 & C22 & C23 & C24 & C25 & C26\\ C31 & C32 & C33 & C34 & C35 & C36\\ C41 & C42 & C43 & C44 & C45 & C46\\ C51 & C52 & C53 & C54 & C55 & C56\\ C61 & C62 & C63 & C64 & C65 & C66\end{pmatrix}\begin{pmatrix}\varepsilon1\\ \varepsilon2\\ \varepsilon3\\ \varepsilon4\\ \varepsilon5\\ \varepsilon6\end{pmatrix} \quad \text{……(3)}$$

And the elastic matrix C_{ij} can be written as[10]:

$$C_{ij} = \begin{bmatrix}C11 & C12 & C13 & C14 & C15 & C16\\ C21 & C22 & C23 & C24 & C25 & C26\\ C31 & C32 & C33 & C34 & C35 & C36\\ C41 & C42 & C43 & C44 & C45 & C46\\ C51 & C52 & C53 & C54 & C55 & C56\\ C61 & C62 & C63 & C64 & C65 & C66\end{bmatrix} \quad \text{…….(4)}$$

Where the elastic matrix of monoclinic Ba_2TiO_4 obtained by Materials studio program and having the values as shown below.

$$C_{ij} = \begin{bmatrix} 53.2241 & 29.1140 & 23.7314 & 0.0000 & 0.0800 & 0.0000\\ 29.1140 & 92.5526 & 38.8026 & 0.0000 & -1.7226 & 0.0000\\ 23.7314 & 38.8026 & 51.6460 & 0.0000 & -0.4849 & 0.0000\\ 0.0000 & 0.0000 & 0.0000 & 11.9197 & 0.0000 & 74.5826\\ 0.0800 & -1.7226 & -.04849 & 0.0000 & 16.3627 & -143.4170\\ 0.0000 & 0.0000 & 0.0000 & 74.5826 & 0.0000 & -143.4170 \end{bmatrix} \quad \text{..(5)}$$

The mechanical stability conditions of the monoclinic Ba_2TiO_4 can be written as[10]:

C11,C22,C33,C44,C55,C55 > 0….(6)

And the condition

(C22+C33 –2C23) > 0…..(7)

According to the mechanical stability conditions the composite is stable mechanically, and this agreed with research[10].The elastic modulus for Ba_2TiO_4 are obtained by Materials studio program using (Reuss model) shown in table 2.

Table 2 .The computed elastic modulus for Ba_2TiO_4 by materials studio MS.

Elastic constant	Symbol	Magnitude	Model
Young modulus	Y	40.29 GPa	Reuss
Shear modulus	G	15.97 GPa	Reuss
Lame coefficient	Λ	142.56 GPa	Reuss
Bulk modulus	B	42.3021 GPa	Reuss
Poisson's ratio	Y	0.3256 GPa	Reuss

The ratio between stress change and corresponding change in strain is called elasticity, provided that the stress is within the limits of elasticity. This ratio is a fixed amount for each material, so it represents the behavior of these materials in relation to the influence of forces on them.. The coefficient of elasticity is defined by the young coefficient, which is denoted (Y)[10]. There is a clearly decrease of the slope (Young modulus) for the aged sample, . The increase in failure strain was also observed for the aged sample, as shown in figure 2 the stress-strain curve representation [11].

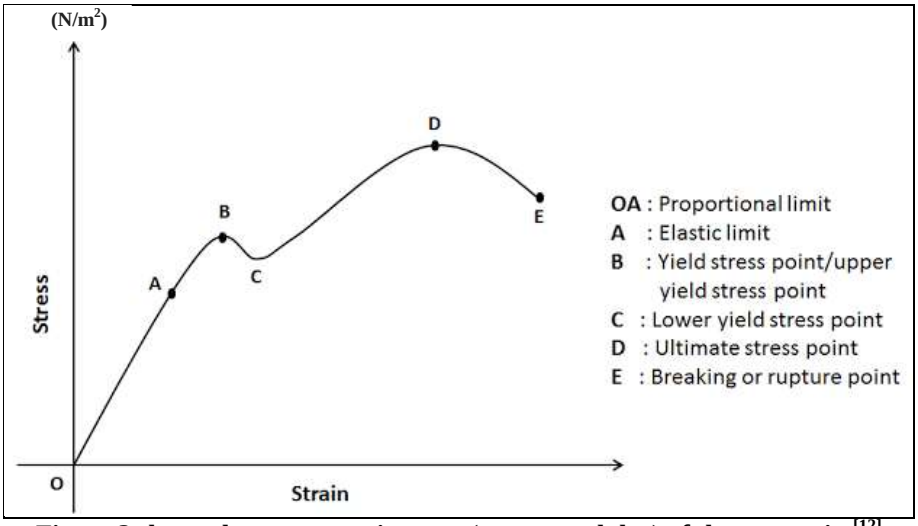


Figure.2 shows the stress–strain curve(young modulus) of the composite[12]

4. Discussion

Some properties where be investigated by theoretical methods using 'the first principles calculations'. The calculated elastic constants as in table.1 and lattice parameters are accessible and comparable values to experimental studies and we have get the convergence of distances between atoms versus optimization step curves from (MS) when we do geometry optimization for the composite as shown in figure 3.

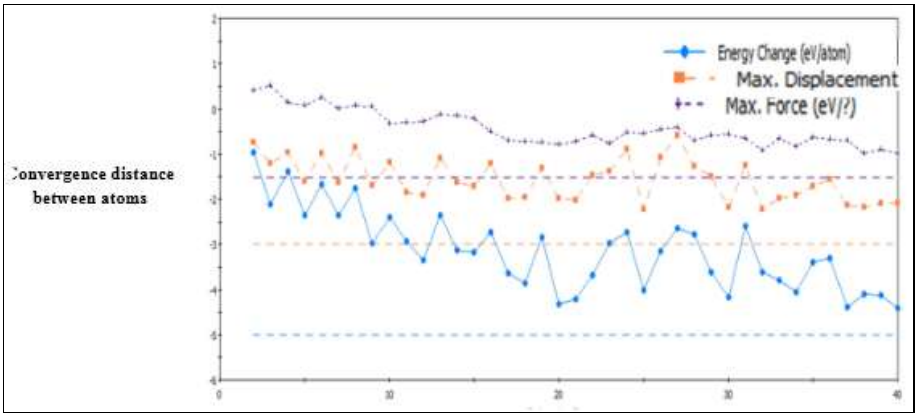


Figure3. Convergence versus geometry optimization

The energy change versus optimization step had been obtained by MS as shown in figure 4 as we see the energy Greatly decreased after optimizing process on the crystalline structure.

ISSN: 1813 – 1662 (Print)
E-ISSN: 2415 – 1726 (On Line)

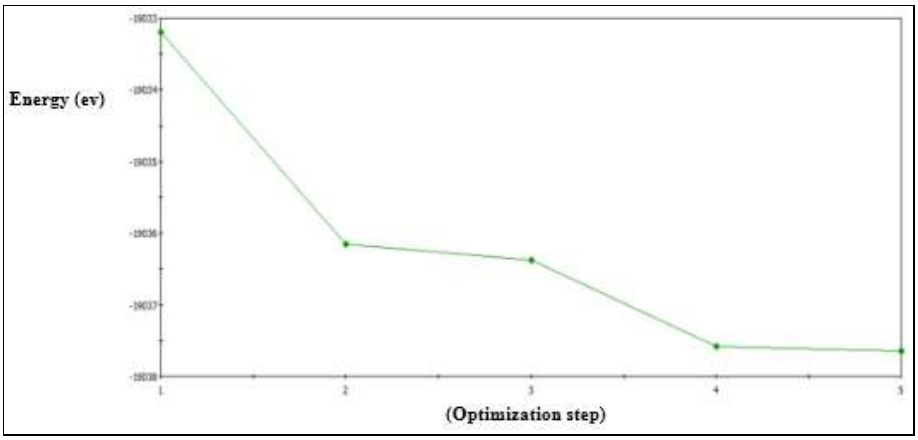


Figure 4. Energy Versus geometry optimization

Density of states is the number of patterns to the frequency unit, calculated by MS is increase as the energy increases shown in figure.5, where the peaks (which represents the energy via density of states) increase as energy increase. The physical meaning of figure5 is that the density of states is increasing versus the energy increase as we can see below in figure 5. Density of states at high level meaning that level is ready for occupation by electrons and density of states at zero level meaning that the level can't be occupied at that level ,as we can see the density of states at high level at Fermi level which means that level is can be occupied by electrons [13].

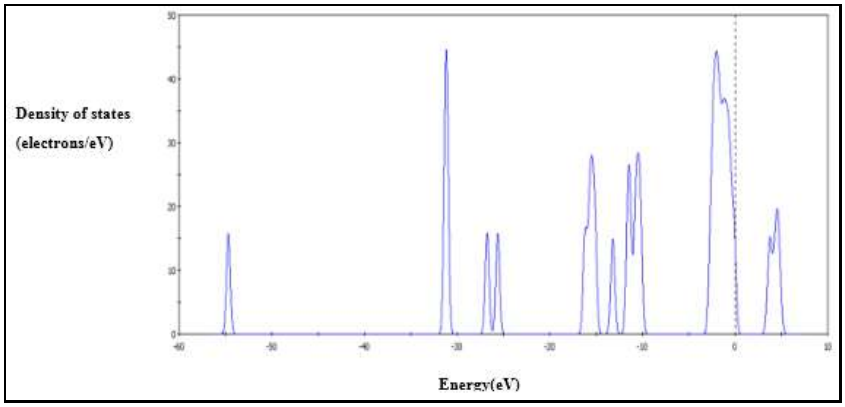


Figure 5 Density of states (DOS)

The band structure of barium orthotitanate having forbidden band gap found equal to Eg = 3.435eV along high symmetry k'-points. these valuewas obtained directly from Materials studio program by applying the simulation steps of the band gap structure, as shown in figure 6 where this value is accessible compared with the other studies and the composite fall in the dielectric range of materials.

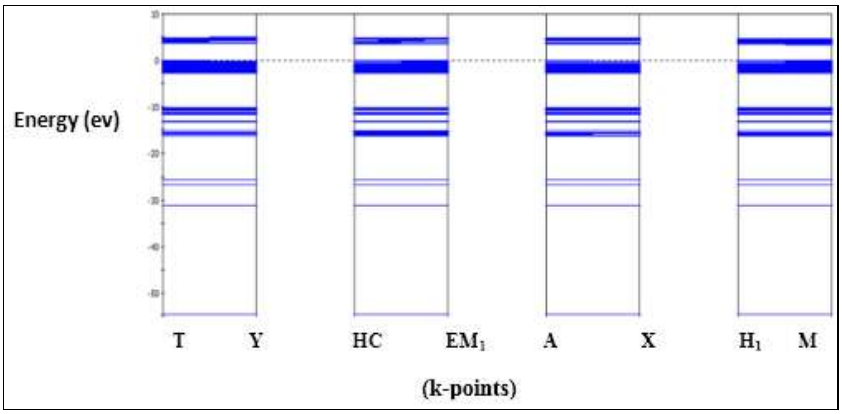


Figure 6 Band structure of Ba_2TiO_4

References

[1] -Yuzhen Mo et al 'Molecular dynamic simulation of the mechanical properties of PI/SiO2 Nano composite based on materials studio', Journal of Chemical and Pharmaceutical Research, 6(6), 1534-1539, (2014).

[2]-J. A. Bland, 'Crystal structure of barium orthotitanate', Journal of Mines and technical surveys, Ottawa, Canada, 14, 875-892, (1961).

[3]- Jon C. Goldsby 'Basic Elastic Properties Predictions of Cubic Cerium Oxide Using First-Principles Methods', *Glenn Research Center, National Aeronautics and Space Administration, 21000 Brook park Road, CleVeland, OH 44135, USA,(2013)*

[4]- Bothina Hamad, 'Ab initio investigations of the structural, electronic, and thermoelectric properties of Fe2NbAl-based alloys, Department of Physics, The University of Jordan, Amman, 51:10887–10896, (2016).

[5]- Dr. rer. Nat' Solid state reactions in electroceramic systems' der Martin - Luther-Universität Halle-Wittenberg. Ukraine, (1980).

[6]-Materials studio software' Materials Science simulation software named Materials Studio, deVeloped by American Accelrys applied in the pharmaceutical,petrochemical, automotive, aerospace industrials and educational research department, (2003).

[7]- Tokeer Ahmad et al, Synthesis of nanometer-sized particles of barium orthotitanate prepared through a modified re Verse micellar route: Structural characterization, phase stability and dielectric properties, J. Mater. Res., Vol. 19, No. 10, Oct (2004).

[8]- American Accelrays ,'Modulus toturial'. San Diego, CA 92121 USA university (2003).

[9]- Ibrahim D. Muhammad et al ' First-Principles Calculations of the Structural, Mechanical and Thermodynamics Properties of Cubic Zirconia', Mechanical Engineering Department, Universiti Teknologi Petronas, Seri Iskandar, Malaysia, 4, 97-103,(2014).

[10]-Ding Ying et al, 'Theoretical investigation on the electronic structure,
elastic properties, and intrinsic hardness of Si2N2Ol' ,Chin. Phys. B, Vol. 21, No. 6 (2012).

[11]- Fabrice Kossi Sodoke et al, Hygrothermal effects on fatigue behavior of quasi-isotropic flax/epoxy composites using principal component analysis', Laboratory of Mechanics and Eco-Materials, Mechanical Engineering Department, University of Quebec at Trois-Rivières, 3351 Boul. des Forges, Trois - Rivières, QC G9A 5H7, Canada (2011).

[12-] B. Civalleri and R. Dovesi, 'Calculation of Equations of State and Elastic Constants, Michigan Tech University USA ,(2009).

[13]-Artur Avila et al, Singular Density of States Measure for Subshift and Quasi-Periodic Schrödinger Operators, Commun. Math. Phys. 330, 469–498 (2014)

نمذجة ومحاكاة الخواص الميكانيكية والفيزيائية لمركب اورثوتيتانات الباريوم Materials Studio بأستخدام برنامج (Ba_2TiO_4)

نجاة احمد دحام[1] ، عبدالله حمود فارس[2] ، خالد عبدالله نجم[1]

[1] قسم الفيزياء ، كلية العلوم ، جامعة تكريت ، تكريت ، العراق

[2] قسم الفيزياء ، كلية التربية للعلوم الصرفة ، جامعة تكريت ، كركوك ، العراق

الملخص

تضمن هذا البحث دراسة الخواص الميكانيكية والخواص الفيزيائية (تركيب حزمة الطاقة, كثافة الحالات) وخواص المرونة لمركب اورثوتيتانات الباريوم (Ba_2TiO_4) , بأستخدام برنامج Materials studio . تمت هذه الحسابات استنادا الى نظرية تقريب التدرج المعمم (GGA), باستخدام حسابات المبادئ الاولى وبطريقة خطية, وكانت قيم ثوابت الشبيكة المحسوبة للنوع احادي الميل كالاتي a = 0.612 nm , c = b = 0.77 nm, وثوابت المرونة المحسوبة للمركب, معامل القص G = 15.97 GP, معامل يونك, فجوة λ= 142.56 GPa, معامل لايم B = 1.05 , ومن خلال هذه القيمة لفجوة الطاقة Eg = 3.435 eV الطاقة ,Y= 40.29 GPa معامل بلوك 42.3021 GPa يكون المركب ضمن المواد العازلة, وتمت هذه الحسابات ضمن مناطق بريليون الاولى, وطبقا لشروط الاستقرارية الميكانيكية Mechanical stability فأن المركب مستقر ميكانيكيا اذ انه يحقق شرط الاستقرارية, وهذه النتائج التي تم الحصول عليها اجريت بأستخدام برنامج Materials studio.

الكلمات الدالة: الديناميكا الجزيئية , الهندسة الامثلية , النمذجة , المحاكاة.