4ème Conférence Internationale des Energies Renouvelables (CIER-2016)
Proceedings of Engineering and Technology – PET
Vol.16, pp.92 - 96

Study of structural and thermal properties of SiO_2 and Al_2O_3 in the Diatomite

K. Boubendira[1,2], K.Labiod[1], S.Benayache[1], A.Benfoughal[1], N.Sassane[1]

[1] *Research Center in Industrial Technologies CRTI, P.O. Box 64, Cheraga Algiers, Algeria*

[2]*Département de Physique, laboratoire de Physique des Rayonnement université Badji mokhtar Annaba, BP 12 Annaba, 23000 Algérie,Name*

[1]K.boubendira@crti.dz

[2]khaled.boub@yahoo.fr

***Abstract*— Diatomite, also known as diatomaceous earth, is the naturally occurring fossilized remains of diatoms. Diatoms are single-celled aquatic algae. They belong to the class of golden brown algae known as Bacillariophyceae. Diatomite is a near pure sedimentary deposit consisting almost entirely of silica. The Greeks first used diatomite over 2,000 years ago in pottery and brick.**

In this work we determine the structural and thermal properties of SiO2 and Al_2O_3 in the diatomite using the plane wave method and linearized augmented (LAPW) in the functional theory of density (DFT).

The potential for exchange and correlation is calculated by the generalized gradient approximation (GGA).

Regarding thermal properties, we calculated the free enthalpy G, S entropy, specific heat C, thermal conductivity λ ..... etc of SiO_2 and Al_2O_3 component. The temperatures used in this work are 1400, 1450 and 1500 respectively;

The results are in good agreement with some experimental data.

***Keywords*— DFT1, Diatomite , thermal proprieties**

I. INTRODUCTION

Still called diatomite kieselguhr is a rock formed by the accumulation in ancient lakes, shells of diatoms are fossil algae amorphous siliceous skeleton. It may be noted industrial and scientific importance of diatomite, quite abundant natural material in Algeria

Diatomite is a well-known natural product, it carries several name; namely: kieselguhr, diatomaceous earth, diatomite, diatomaceous earth, tripoli, and diatomaceous flour.

This is a clear colored rock consisting primarily of silica and impurities (organic compounds, sand, clay, calcium carbonate and magnesium, salts, ...). These unicellular algae are surrounded by a silica shell [1].

The crystalline SiO_2 is transparent to visible light because of the wide band gap between the valence band and the conduction band (eg, the band interval is ~ 10eV for α-quartz [2-3]). A similar behavior is observed in amorphous SiO_2, which is the main component of window glasses. With the presence of dopants, people can dramatically change the optical absorption properties of SiO_2 in the visible range. One of the most commonly used methods is the co-doping of Al_2O_3 with rare earth elements (for example, Nd, Er) to SiO_2 and the doped SiO_2 appears to have interesting optical and spectroscopic properties, new absorption peaks are observed in the infrared and visible range.[4-6].

Al_2O_3 dopants have been shown to play an important role in the geometric distribution of rare earth elements,

To prevent the regrouping of rare earth ions, which in turn reform the quality of optical devices [6]. Numerous experiments have been carried out to study the number of oxygen coordination (OCN) of the Al atoms in the SiO_2 glass and their melts at high temperature. Using electronic paramagnetic resonance (EPR), people have established that Al atoms are more likely to substitute Si positions in natural quartz [7-9].

Alumina (aluminum oxide) is a ceramic material of great interest, both for fundamental studies and for applications. It is a material of considerable technological and industrial importance due to its hardness, abrasion resistance, mechanical strength, corrosion resistance, good electrical insulation, its properties Optical properties [10], its fine particle size, its specific surface area and its catalytic surface activity. Its melting point and its electrical conductivity are respectively 2327 K and 10-12 s / m at 20°C. Alumina or Al_2O_3 has a number of different phases, such as α, β, γ, κ, η, θ and al alumina. The electronic structure of alumina (Al_2O_3) is increasingly interesting for its variety of applications in optical, electronic and structural devices. For example, α-Al_2O_3 is used in electronics, the γ phase in catalysts and the κ phase in the wear-resistant coating on cemented carbide cutting tools [11-13]. Unlike the α-Al_2O_3 phase, whose structure has been known for a long time, only a few experimental and theoretical studies have been carried out on κ-Al_2O_3. The difficulty of obtaining significant amounts of a pure sample of κ-Al_2O_3 and the low degree of crystallinity hampered the experimental determination of its electrical and optical properties [14].

ISSN 2356-5608

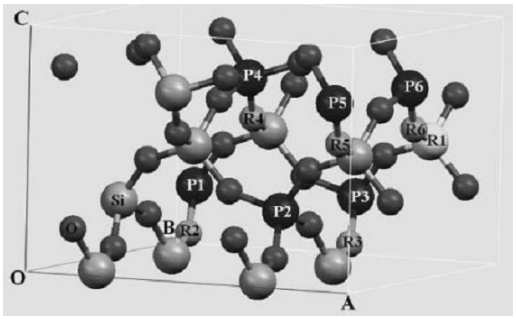

Fig. 1 Atomic bonding structure of the SiO2 crystal (α-cristobalite, 2x2x1unit cell). The Si atoms are represented by large (grey) balls, and the O atoms are represented by small (red) balls [3].

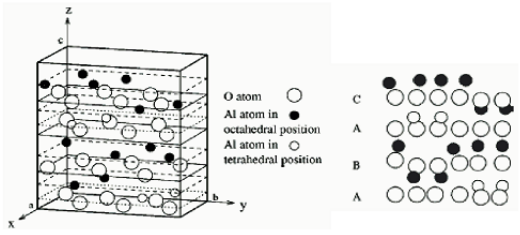

FIG. 2: Crystal structure and atomic position of κ-Al2O3 [15]

II. METHOD OF CALCULATION

The calculation of the structural and thermal properties of Al_2O_3 and SiO_2 was carried out with a self-consistent scheme by solving the Kohn-Sham equations, using a FP-LAPW method in the framework of the density functional theory (DFT), along with the generalized gradient approximation (GGA) method [16 - 19] using the Wien2k codes [20]. The calculation was performed with 3000 k-points and Rk_{max}= 7 (R is the smallest muffin-tin radius and k_{max} is the cut-off wave vector of the plane-wave basis set) for the convergence parameter, for which the calculation stabilizes and convergence in terms of the energy is achieved. The values of the other parameters are G_{max}= 14 a_0^{-1} (G_{max} is the magnitude of the largest vector in the charge density Fourier expansion or the plane wave cutoff, and a_0 is the Bohr radius), R_{MT} (Al)=1.6 au, (Si)= 1.56 au, and R_{MT} (O)=1.7 au (muffin-tinradius). The iteration was halted when the difference charge density was less than 0.00001e a_0^{-1} between steps, taken as a convergence criterion. The core cut off energy, which defines the separation of core and valence states, was chosen as −8 Ry. The cell parameters obtained for the two systems are listed in TABLE I

III. RESULTS

TABLE I
CRYSTAL PARAMETER OF SiO_2 AND AL_2O_3

	a (A°)	B (A°)	C (A°)	α (°)	β (°)	γ (°)
SiO_2						
Calculation	5.019	5.019	6.989	90.00	90.00	90.00
[1]Experiment	4.971	4.971	6.922	90.00	90.00	90.00
[2]Other calcs	5.053	5.053	7.037	90.00	90.00	90.00
Al_2O_3						
Calculation	4.842	8.357	8.962	90.00	90.00	90.00
[3]Experiment	4.835	8.310	8.936	90.00	90.00	90.00
[4]Other calcs	4.843	8.222	9.001	90.00	90.00	90.00

[1]Ref.[21], [2]Ref.[3], [3]Ref.[22], [4]Ref.[10]

IV. CALCULATION OF THERMAL PROPERTIES OF AL_2O_3 AND SiO_2

According to data available on this product "diatomite"; and in the characterization that has been made, especially the chemical analysis of the diatomite sample recovered from the Diatal unit (subsidiary of ENOF group, Algeria) and was analyzed by XRF spectrometry [1,2] our product consists of the following elements, summarized in TABLE II.

TABLE II
ANALYSIS OF CHEMICAL COMPOSITION OF DIATOMITE POWDER

MgO	Fe_2O_3	TiO_2	CaO	K_2O	SiO_2	Al_2O_3	Na_2O
2.15	1.29	0.027	13.4	0.79	60.4	3.156	1.2

Calculating the thermal properties of each element was made using WIEN2k code [20]. To make these calculations we used two temperature values 1450 and 1500 ° C respectively, for a pressure value 1 GPa.

The results obtained (Al_2O_3 and SiO_2 in diatomite) are presented in the following TABLES:

for Al_2O_3

TABLE III
A THERMAL PROPERTIES OF AL_2O_3, SUCH AS DEBYE TEMPERATURE (THETA) , HEAT CAPACITY C_V AND THE THERMAL EXPANSION COEFFICIENT (ALPHA) … ETC; AT A TEMPERATURE OF T = 1450 °C AND PRESSURE: P = 1 GPA

numerical equilibrium, vibrational, properties and thermal eos derivatives				
G (kJ/mo)	V (bohr3)	U (kJ/mol)	A (kJ/mol)	S (J/mol*K)
-96.92	167.52	72.62	-115.60	129.81

ISSN 2356-5608

numerical equilibrium, vibrational, properties and thermal eos derivatives			
Theta (K)	Alpha (10^5/K)	C (J/Kg.°C)	λ (W/m.K)
394.05	10.562	3252.71	0.085

TABLE IV
A THERMAL PROPERTIES OF Al_2O_3, SUCH AS DEBYE TEMPERATURE (THETA) , HEAT CAPACITY C_V AND THE THERMAL EXPANSION COEFFICIENT (ALPHA) … ETC; AT A TEMPERATURE OF T = 1500 °C AND PRESSURE: P = 1 GPA

numerical equilibrium, vibrational, properties and thermal eos derivatives				
G (kJ/mo)	V (bohr3)	U (kJ/mol)	A (kJ/mol)	S (J/mol*K)
-103.47	168.47	75.10	-122.97	132.047

numerical equilibrium, vibrational, properties and thermal eos derivatives			
Theta (K)	Alpha (10^5/K)	C (J/Kg.°C)	λ (W/m.K)
404.01	10.538	3258.81	0.053

for SiO_2

TABLE V
A THERMAL PROPERTIES OF SiO_2, SUCH AS DEBYE TEMPERATURE (THETA) , HEAT CAPACITY C_V AND THE THERMAL EXPANSION COEFFICIENT (ALPHA) … ETC; AT A TEMPERATURE OF T = 1450 °C AND PRESSURE: P = 1 GPA

numerical equilibrium, vibrational, properties and thermal eos derivatives				
G (kJ/mo)	V (bohr3)	U (kJ/mol)	A (kJ/mol)	S (J/mol*K)
-71.82	114.56	58.63	-105.63	112.61

numerical equilibrium, vibrational, properties and thermal eos derivatives			
Theta (K)	Alpha (10^5/K)	C (J/Kg.°C)	λ (W/m.K)
398.54	9.876	3251.699	0.080

TABLE VI
A THERMAL PROPERTIES OF SiO_2, SUCH AS DEBYE TEMPERATURE (THETA) , HEAT CAPACITY C_V AND THE THERMAL EXPANSION COEFFICIENT (ALPHA) … ETC; AT A TEMPERATURE OF T = 1500 °C AND PRESSURE: P = 1 GPA

numerical equilibrium, vibrational, properties and thermal eos derivatives				
G (kJ/mo)	V (bohr3)	U (kJ/mol)	A (kJ/mol)	S (J/mol*K)
-80.49	118.41	63.17	-112.95	119.097

numerical equilibrium, vibrational, properties and thermal eos derivatives			
Theta (K)	Alpha (10^5/K)	C (J/Kg.°C)	λ (W/m.K)
408.54	9.876	3259.56	0.051

V. CONCLUSIONS

This work is part of research projects URMA / CRTI 'recovery ceramics.

In this work we calculated the structural and thermal properties of Al_2O_3 and SiO_2 in the diatomite product; such as G, S, C, ... etc. λ.

Concerning structural properties:

- The computed lattice constants of the Al2O3 and SiO2 are in reasonable agreement with available theoretical and experimental data,

For thermal properties:

- The Al_2O_3 and SiO_2 simulation results in diatomite are shown in the tables above.

According to some experimental data especially related to the thermal conductivity "λ" and Specific heat "C" (reference [1] and [23]); it can be seen that our simulation results are very close to those of experiment.

ISSN 2356-5608

REFERENCES

[1] Hazem MERADI, L. ATOUI, A. Balaska, S. BOUHOUCHE, « Contribution à la caractérisation d'une diatomite naturelle ». 9ième Congrès de Mécanique, FS Semlalia, Marrakech du 21 au 24 Avril 2009.

[2] E. K. Chang, M. Rohlfing and S. G. Louie: Phys. Rev. Lett.85(2000) 2613.

[3] Yong Yang, Masae Takahashi, and all, Structural, Electronic and Optical Properties of the Al2O3Doped SiO2:First Principles Calculations, Materials Transactions, Vol. 49, No. 11,p2474, 2008.

[4] M. G. Ferreira da Silva: J. Non-Cryst. Solids 352, 807.2006.

[5] S. Berneschi, M. Bettinelli, M. Brenci, G. N. Conti, S. Pelli, S. Sebastiani, C. Siligardi, A. Speghini and G. C. Righini: J. Non-Cryst. Solids351, 1747.2005.

[6] S. Sen and J. F. Stebbins: J. Non-Cryst. Solids188, 54.1995.

[7] R. H. D. Nuttall and J. A. Weil: Can. J. Phys.59, 1696. 1981.

[8] R. S. Dickson and J. A. Weil: Can. J. Phys.68, 630. 1990.

[9] D. F. Howarth, M. J. Mombourquette and J. A. Weil: Can. J. Phys.75, 99. 1997.

[10] S. J. Mousavi, S. M. Hosseini and all, Calculation of the Structural, Electrical, and Optical Properties of κ-Al_2O_3 by Density Functional Theory,46, 2. 2008.

[11] R. H. French, J. Am. Ceram. Soc. 73, 477. 1990.

[12] M. V. Finnis, J. Phys.: Condens. Matter 8, 5811. 1996.

[13] D. G. Cahilla, S. M. Lee, and T. I. Selinder, J. Appl. Phys. 83, 5783. 1998.

[14] H. L. Gross and W. Mader, Chem. Commun., 55–60. 1997.

[15] B. Holm, R. Ahuja, Y. Yourdshahyan, B. Johansson, and B. I. Lundqvist, Phys. Rev. B 59,12777. 1999.

[16] K. Schwarz, J. Sol. St. Chem. 176, 319. 2003.

[17] K. Schwarz, P. Blaha, Comput. Mat. Sci. 28, 259. 2003.

[18] K. Schwarz, P. Blaha, G. K. H. Madsen, Comput. Phys. Comm un. 147, 71. 2002.

[19] M. Peterson et al., Comput. Phys. Commun., 126, 294. 2000.

[20] P. Blaha, K. Schwarz, G. Madsen, D. Kvasnicka, and J. Luitz, Inst. F. Mat. Chem., TU Vienna, http://www.wien2k.at/

[21] R. T. Downs and D. C. Palmer: Am. Mineral.79, 9. 1994.

[22] B. Ollivier, R. Retoux, P. Lacorre, D. Massiot, and G. Ferey, Mater. Chem. 7, 1049. 1997.

[23] Redouan NAKKAD, Hassan EZBAKHE, Abdelkhalak BENMOUSSA, Taïb AJZOUL et Abderrahman EL BAKKOURI, « contribution à l'etude morphologique et thermique des diatomites utilisees dans l'isolation », 12èmes Journées Internationales de Thermique, Tanger, Maroc du 15 au 17 Novembre 2005.

ISSN 2356-5608