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Research Article

Study of Structural and Thermal Properties of SiO2 and MgO in the Diatomite[#]

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Abstract: The diatomite still called kieselguhr is a rock formed by accumulation in old lakes, carapaces of diatoms which are fossil algae with siliceous skeleton amorphous and slightly hydrated. The diatoms are very abundant and there are several species corresponding to species different of diatomite. In this work we determine the structural and thermal properties of SiO_2 and MgO 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). For the thermal properties, we calculated the free enthalpy G, S entropy, specific heat C, thermal conductivity λ ..... etc of SiO_2 and MgO component. The temperatures used in this work are 1400, 1450 and 1500 respectively;The results are in good agreement with some experimental data.

1. 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]) (Fig. 1). 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, 5, 6].

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

The alkaline-earth chalcogenides MgO compound has a NaCl crystal structure. The valence band of this compound is formed by hybridized O 2p and S 3p states, respectively, while the bottom of the conduction band is commonly associated with Mg 3s states [7]. Alkaline-earth metal oxides are technologically important materials applied in medicine, heterogeneous catalysis, and electronics [8].

MgO is a II-VI semiconducting material with a wide band gap. Its alloys have been increasingly investigated due to a UV luminescence ranging from 150 to 400 nm or alternatively wide band gaps from 3.3 to 7.8 eV [9]. Nanostructure materials are

investigated for their potential applications in photovoltaic, electrooptical, micromechanical, and sensor devices [10]. Mobile phones, satellites, fiber optic data transmission systems, and other advanced technologies such as laser diodes and magnetic detectors are expanding throughout the world, and are transforming our everyday lives. (Fig. 2).

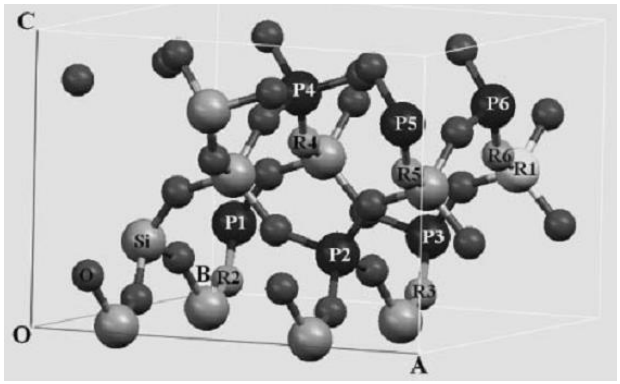

Figure 1. *Atomic bonding structure of the SiO_2 crystal (α-cristobalite, 2x2x1unit cell). The Si atoms are represented by large (grey) balls, and the O atoms are represented by small (black) balls [3].*

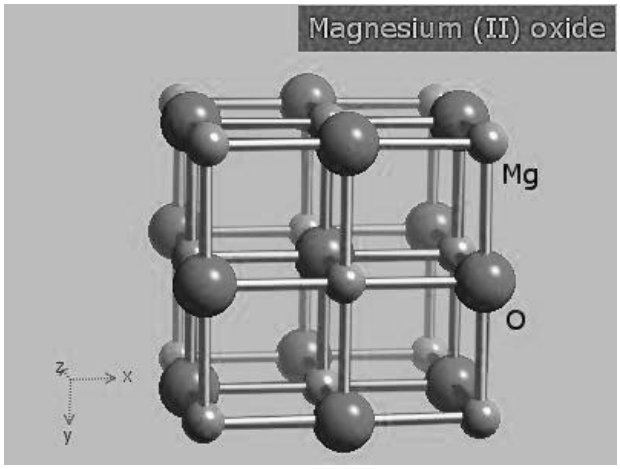

Figure 2. *Atomic bonding structure of the MgO crystal. The O atoms are represented by large balls, and the Mg atoms are represented by small balls [2].*

2. Method of calculatıon

The calculation of the structural and thermal properties of MgO and SiO2 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 [11, 12, 13, 14] using the Wien2k codes [15]. The calculation was performed with 3000 k-points and Rkmax= 7 (R is the smallest muffin-tin radius and kmax 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 Gmax= 14 a0-1 (Gmax is the magnitude of the largest vector in the charge density Fourier expansion or the plane wave cutoff, and a0 is the Bohr radius), RMT (Mg)=2.1 au, (Si)= 1.56 au, and RMT (O)=1.7 au (muffin-tinradius). The iteration was halted when the difference charge density was less than 0.00001 e 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 1.

Table 1 *Crystal parameter of SiO_2 and MgO*

	a(A°)	*b(A°)*	*c(A°)*	*A= β= γ(°)*
SiO_2				
Calculation	5.019	5.019	6.989	90.00
[1]Experiment	4.971	4.971	6.922	90.00
[2]Other calcul.	5.053	5.053	7.037	90.00
MgO	a=b=c			
Calculation	4.196			90.00
[3]Experiment	4.212			90.00
[4]Other calcul.	4.259			90.00

[1]Ref.[16], [2]Ref.[3], [3]Ref.[17], [4]Ref.[18]

3. Results

3.1. Calculatıon of thermal propertıes of MgO 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] our product consists of the following elements, summarized in table 2.

Calculating the thermal properties of each element was made using WIEN2k code [15]. To make these calculations we used two temperature values 1450 and 1500 ° C respectively, for a pressure value 1 GPa.

The results obtained (MgO and SiO2 in diatomite) are presented in the following Tables 3-6.

4.Conclusions

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

In this work we calculated the structural and thermal properties of MgO and SiO2 in the diatomite product; such as G, S, C, ... etc. λ.

Concerning structural properties:

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

For thermal properties:

- The MgO and SiO2 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 [19]); it can be seen that our simulation results are very close to those of experiment.

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The authors' responsibilities were as follows- Boubendira: designed the research and wrote the manuscript;

Boubendira and K.Labiod: analyzed data; S.Benayache, F.Aoudja, A.Benfoughal and N.Sassane: edited the manuscript;

Boubendira: conducted the research and had primary responsibility for the final content of the manuscript; and all authors: read and approved the final manuscript. none of the authors had a conflict of interest.

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Table 2 *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

Table 3 *A thermal properties of MgO, such as Debye temperature (Theta) , heat capacity C 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)	Theta (K)	Alpha (10^5/K)	C (J/Kg.°C)	λ (W/m.K)
3.95	167.09	36.56	-11.70	63.94	682.48	5.308	3261.88	0.059

Table 4. *A thermal properties of MgO, such as Debye temperature (Theta) , heat capacity C 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)	Theta (K)	Alpha (10^5/K)	C (J/Kg.°C)	λ (W/m.K)
0.42	167.54	38.93	-15.42	70.47	679.11	5.332	3259.45	0.06

Table 5 *A thermal properties of SiO_2, such as Debye temperature (Theta) , heat capacity C 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)	Theta (K)	Alpha (10^5/K)	C (J/Kg.°C)	λ (W/m.K)
-71.82	114.56	58.63	-105.63	112.61	398.54	9.876	3251.699	0.080

Table 6 *A thermal properties of SiO_2, such as Debye temperature (Theta) , heat capacity C 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)	Theta (K)	Alpha (10^5/K)	C (J/Kg.°C)	λ (W/m.K)
-80.49	118.41	63.17	-112.95	119.097	394.05	10.562	3252.71	0.085