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Body Wave Velocities and Azimuthal Seismic Anisotropy of Nanostructure Polymorphs of Silica under High Pressure

Saliha Belabas[1], Khalissa Layadi[2], Zohir Radi[2,3*], and Mahmoud Hamlaoui[4]

[1]*Département Physique Faculté des Sciences Université Ferhat Abbas Sétif.*
[2]*Center for Research in Astronomy, Astrophysics and Geophysics.*
[3]*Laboratory for Studies of Surfaces and Interfaces of Solid Materials (LESIMS), Ferhat Abbas University, Sétif, Algeria.*
[4]*Institut d'Architecture et Science de la Terre, Ferhat Abbas University, Sétif, Algeria.*

**(zohir.radi@craag.edu.dz)*

Abstract – In this study, the elastic body wave velocities and seismic anisotropy of two high-pressure polymorphs of silica, stishovite and $CaCl_2$-type, are obtained in 0-80 GPa of earth's pressure mantle at zero temperature from their elastic constants tensor. This last were obtained previously using Density Functional Theory in 0-80 GPa based on reducing an interacting many-electron problem to a single-electron problem by Radi et al. (2023b). In order to estimate the theoretical V_P and Vs in 0-80 GPa of the two polymorphs of SiO_2, we considered the results of Radi et al. (2023b) dependence of bulk modulus, shear modulus, and density with pressure. Our obtained results of seismic wave velocities showed that Vs varies very little with pressure, from 7.1 (at 10 GPa) to 7.9 (at 80 GPa) km/s, whereas the variation of V_P is significant, ranges from 11.5 to 13.5 km/s. The azimuthal anisotropy variation showed that S-wave is strongly anisotropic than P-wave, with a decrease of 60 and 10% at 40 GPa phase transition pressure defined previously by Radi et al. (2023b) using the Gibbs free energy formulas and enthalpy difference results. Our obtained results may be relevant in understanding the deep Earth structure from the geophysical implication of the stishovite and $CaCl_2$-type transformation.

Keywords – High-Pressure; Elastic Body Wave; Azimuthal Anisotropy; Stishovite; $CaCl_2$-Type; SiO_2

I. INTRODUCTİON

Silicon (Si) and Oxygen (O) are the two most common chemical elements in the earth's crust and mantle. Therefore, it is not surprising that a group of minerals composed basically of these two elements with a number of other ions and named silica, SiO_2, takes on several structural arrangements (SiO_2 is considered the most chemical element in the primitive mantle or bulk

The Silicate Earth; composition, 46 wt %, from [1]). High pressure and temperature have a great role in the stability of the elastic properties of the major materials of the earth's mantle. The high-pressure behavior of these properties can be determined by theoretical methods with certain limitations. There are six different crystalline forms of transformation depending on the pressure ranging from 0 to 300 GPa: quartz, coesite, stishovite, CaCl2-type, seifertite (α-PbO_2-type), and pyrite [2]. According to [3], the Earth's crust [2] upper mantle is mainly composed of SiO_2, coming from rocks of the Earth's surface sinking into the lower mantle. This mineral is minor in extraterrestrial materials [4].

II. MATERİALS AND METHOD

In our application of DFT, the Cambridge Serial Total Energy Package (CASTEP) code is used ([5, 6]). It can give information on the total energies, and forces, and insists on an atomic system, as well as the calculation of optimal geometries, band structures, optical spectra…We used the pseudo-potential approximation, plane wave function, and the Monkhorst-Pack scheme to reduce the number of variables and sample the irreducible Brillouin zone ([7]). In the present study, we took a Brillouin zone at the special k-points generated by a sampling grid of 8x8x8 and a wave plane energy cut-off equal to 450 eV, to obtain a good convergence of the calculations for reliable results. The fully optimized structure of stishovite and $CaCl_2$-type phases of silica was used to determine the elastic proprieties, which allows refining the geometry of a 3D periodic system to obtain a stable structure or polymorph. Pressure dependence of the volume, density, elastic constants were given as curves with some fundamental formulas.

III. RESULTS

Results In this study, we used theoretical calculations for $T = 0$ K, so $G = Ettt + P * V$. The enthalpy of formation of each structure (stishovite or CaCl2-type phase) was calculated for several pressure values (Fig. 1). At each ressure, the stishovite's enthalpy value is taken as the reference and the difference between both phases is presented as the value of the enthalpy of formation of the second phase.

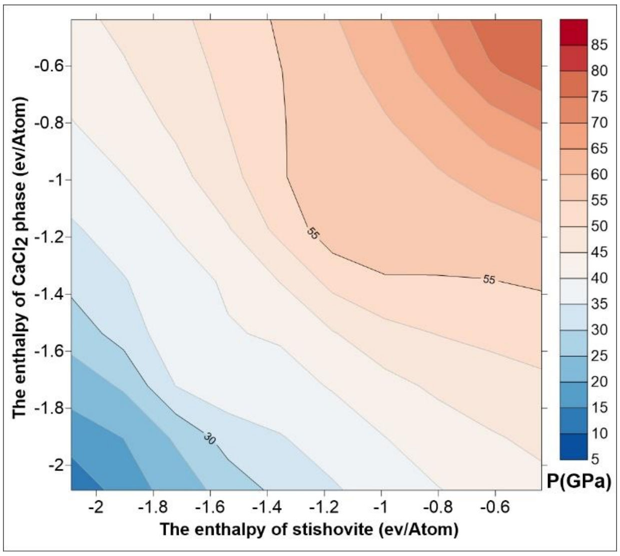

Fig. 1. The enthalpy of stishovite and $CaCl_2$-type phases as a function of pressure.

The bulk modulus, B, represents the resistance of the crystal during the application of the constraints, to preserve its volume, whereas the shear modulus, G, which represents the resistance to plastic deformation.

IV. CONCLUSION

From the stishovite seismic anisotropy analysis, it is clear that there is a 26% variation in V_P and a 109.5% variation in Vs. If silica exists freely in the lower mantle, this indicates that there is an observable seismic discontinuity in the lower

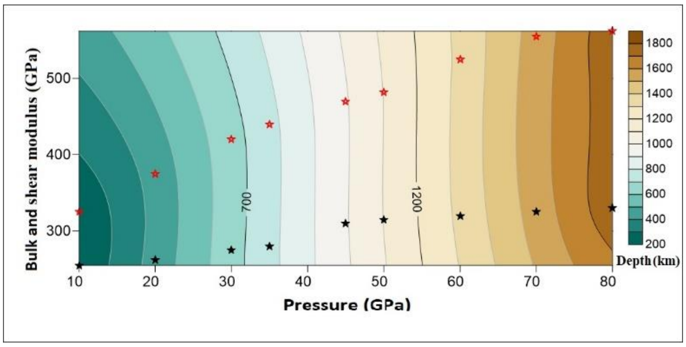

Fig. 2. The variation of bulk modulus, BB, and shear modulus, GG, as a function of pressure for SiO_2 for stishovite (0 to 40 GPa) and $CaCl_2$-type (40 to 80 GPa).

V. DISCUSSION

The isotropic body waves were calculated from the high-pressure dependence of the bulk modulus, B, shear modulus G, and density, ρ obtained by [8] (submitted) , using the relationships n° 01 and 02.

$$V_P = \sqrt{(B + \tfrac{4}{3}G)/\rho}. \quad (1)$$

$$V_s = \sqrt{G/\rho} \quad (2)$$

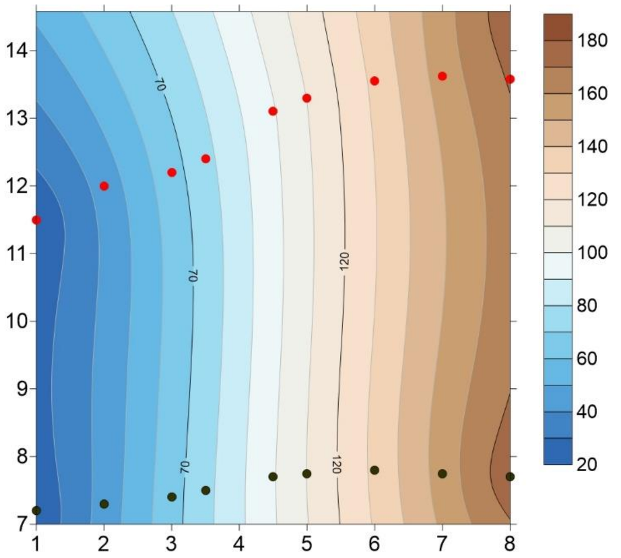

Fig. 3: The P wave and S wave velocities obtained in the present study.

mantle at 40 GPa which corresponds to a depth of ~1000 km. Our calculations for geophysical implication and previous studies considering the temperature in the pressure phase transition of stishovite-$CaCl_2$-type showed that the 1000-2000 km zone in the lower mantle contains free silicate. The method followed in the present study allows us to study a pure pole in the lower mantle, SiO_2. This method will enable us to study the other oxides by determining their elastic properties to give tomographic images, representing the variation of seismic velocities in Earth's layers exp [9], [10] and [11].

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REFERENCES

[1] Condie K.C., Academic Press, 2011.

[2] Stishov S.M., Popova S.V., 10, 839 - 937, 1961; https://doi.org/10.4269/ajtmh.1961.10.839

[3] Kayama, M., Nagaoka, H.; and TNiihara, T. Minerals 2018, 8, 267;M. Wegmuller, J. P. von der Weid, P. Oberson, and N. Gisin, "High resolution fiber distributed measurements with coherent OFDR," in *Proc. ECOC'00*, 2000, paper 11.3.4, p. 109.

[4] R. E. Sorace, V. S. Reinhardt, and S. A. Vaughn, "High-speed digital-to-RF converter," U.S. Patent 5 668 842, Sept. 16, 1997.

[5] Segall M.D., Lindan P.J.D., Probert M.J., Pickard C.J., Hasnip P.J., Clark S.J., Payne M.C., J.Phys,Lett, 14, p 2717, 2002 ; https://doi.org/10.1088/0953-8984/14/11/301

[6] Clark Stewart J., Segall Matthew D., Pickard Chris J., Hasnip Phil J., Probert Matt I. J., Keith Refson and Payne Mike C. ; https://doi.org/10.1524/zkri.220.5.567.65075

[7] Payne J.W.,Bettman J.R., Schkade D.A., Fuqua School of Busi, 1998. "PDCA12-70 data sheet," Opto Speed SA, Mezzovico, Switzerland.

[8] Tsuchiya T., Caracas R., Tsuchiya J., Geophysical Research Letters, 31, L11610, 2004; https://doi.org/10.1029/2004GL019649.

[9] Radi. Z. Étude de l'anisotropie sismique du nord-Est de l'Algérie. http://dspace.univ-setif.dz:8888/jspui/handle/123456789/1584.

[10] Radi Z., and A.K. Yelles-Chaouche, Shear velocity structure beneath Northern Algeria from Rayleigh-wave analysis, J. African Earth Sci. 186, 104446, 2022.

[11] Radi, Z., S. Tlili, K. Layadi, L. Louail, A. Yells-Chaouche, Y. Madhekour, S. Guettouche. Elastic Proprieties of SiO2 nanostructure in High-Pressure Condition, Vol.18,No. 1, January - March 2023, p. 273 - 278. DOI: 10.15251/DJNB.2023. 181.273.