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Elastic Properties of Mantle Minerals at Different Temperatures

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ABSTRACT;

The elastic properties of mantle minerals are important for the interpretation of the structure and composition of the lower mantle. In the present work we have calculated the elastic mouli such as bulk modulus, Young's modulus and shear modulus for Al_2O_3 & MgO to study their ductility and brittleness at different temperature ranges by using Hill's averaging method and other methods of thermodynamics. The fracture / toughness ratio increases with the temperature for Al_2O_3 (>1.75) & MgO (<1.75). On the basis of these results it is clear that the nature of Al_2O_3 is ductile whereas MgO is brittle in nature.

Key Words: Mantle minerals, elastic properties, fracture / toughness, ductility and brittleness.

INTRODUCTION:

Elastic properties of mantle minerals are closely related to many fundamental properties and their variation with temperature provide useful knowledge about nature of interatomic forces. The elastic properties of minerals depend on its composition, crystal structure, temperature and the level of defect. It is of current interest to the geophysicists and scientists because it is severely required in the analysis of geochemical and geophysical problems. The thermo elastic properties of minerals at high temperature (T) and pressure (P) provides an opportunity for understanding the characteristic behavior of deep Earth's interior. Among the several relations correlating shear modulus G, and single-crystal elastic coefficients C_{ij} , the most well known theoretical relations define the effective isotropic shear modulus in terms of the single-crystal elastic moduli through the upper and lower bounds[1-3]. The elastic properties of solids also provides a path to study the mechanical properties such as brittleness and ductility of solids for their technological applications in different fields of engineering and science. Since the adiabatic bulk modulus (K) and shear modulus (G) represents the resistance to fracture and plastic deformation respectively, therefore the ratio K/G will be an indication of ductile or brittle characters. The ratio K/G decides the brittleness and ductile behavior of material when the ratio of resistance to fracture and plastic deformation is greater than 1.75 (i.e. $K/G > 1.75$) material behaves as ductile material whereas if $K/G < 1.75$ it behaves as brittle material.

In this work a simple and straight forward model theory Hill's averaging method [4] is used to analyze the elastic properties of two geophysical minerals viz. Al_2O_3 and MgO.

THEORY;

Under uniform stress for an isotropic elastic medium the crystal holds the fundamental principles of elastic stress-strain relation. For isotropic solids the quantities Y (Young's Modulus), G (Shear modulus) and σ (Poisson's ratio) satisfy the relation [5].

$$G = \frac{Y}{2(\sigma + 1)} \quad (1)$$

For solids the Bulk modulus of elasticity in terms of elastic stiffness coefficients [2, 3] is given as-

$$K = \frac{C_{11} + 2C_{12}}{3} \quad (2)$$

where C_{11} and C_{12} are function of applied pressure (P).

Cauchy's relationship [4, 5] is given by

$$C_{12} - C_{44} = 2P \quad (3)$$

The two shear constants [4, 5] can be written as;

$$C_s = \frac{3}{4}(C_{11} - K)$$

and $C_{44} = \frac{3}{2}K - \frac{1}{2}C_{11} - 2P$

The value of G used is the arithmetic mean called the Hill Average G = ½ ($G^V + G^R$) Here we present Hill's averaging method, the average of the upper bound (superscript V) and the lower bound (superscript R), because it is less complicated. The average isotropic shear modulus G is found from G^V and G^R given as;

$G^V = 1/5\ (2C_S + 3C_{44}) = 3/5(K-2P)$

& $G^R = [1/5(2/C_S + 3/C_{44})]^{-1}$

$$G = ½\ (G^V + G^R) \quad (4)$$

The valve of Poisson's ratio [4,5] is given as;

$$\sigma = \frac{3 - \left(\frac{2G}{K}\right)}{2\left[3 + \frac{G}{K}\right]} \quad (5)$$

RESULTS AND DISCUSSION;

In this work averaging method introduced by Hill's and other different expressions are used to calculate the elastic coefficients for two geophysical minerals viz. Al_2O_3 and MgO at different temperatures. The elastic parameters such as Y, K, P, G and σ for the selected minerals are calculated by using the equations (1), (2), (3), (4) and (5) respectively. For these calculations input values of elastic coefficients are taken from table-1. The calculated values of σ and K/G for MgO and Al_2O_3 are displayed in table-2 and table-3 respectively. From the analysis of data given in table it is found that elastic coefficients (Y, K and G) as usual decreases with increasing temperature, the Poisson's ratio remains almost constant for a wide ranges of temperatures [6]. The fracture / toughness ratio increases with the temperature for Al_2O_3 and MgO. The experimental evidences reveal that the substances having K/G ratio greater than 1.75 are ductile in nature whereas if the K/G ratio are less than 1.75 the substance will brittle in nature. On the basis of calculated values of K/G ratio given in the table it is clear that the nature of Al_2O_3 is ductile whereas MgO is brittle in nature.

Table-1: Input parameters (Elastic stiffness coefficients) at different temperatures for Al_2O_3 and MgO [7]

	Al_2O_3			MgO		
T(K)	**C_{11}**	**C_{12}**	**C_{44}**	**C_{11}**	**C_{12}**	**C_{44}**
300	497.2	162.8	146.7	299	96.4	157.1
400	494.7	163.8	144.4	292	97	155.8
500	490.6	163.7	141.8	286.9	97.6	154.3
600	486	163.1	139.2	280.6	98	152.8
700	481.5	162.9	136.5	274.5	98.4	151.3
800	476.8	162.4	133.9	268.2	98.5	149.7
900	472.3	162.4	131.2	261.9	98.6	148.1
1000	467.4	161.4	128.6	255.7	98.7	146.5

Table-2: Calculated values of Shear modulus (G in GPa), Bulk modulus (K in GPa), Young's modulus (Y in GPa), Poisson's ratio (σ) and Fracture/Toughness ratio (K/G) for Al_2O_3 at different temperatures

T(K)	**G**	**K**	**Y**	**σ**	**K/G**
300	154.58	274.27	390.40	0.26	1.77
400	152.48	274.10	385.89	0.27	1.80
500	150.10	272.67	380.47	0.27	1.82
600	147.71	270.73	374.94	0.27	1.83
700	145.20	269.10	369.21	0.27	1.85
800	142.78	267.20	363.58	0.27	1.87
900	140.23	265.70	357.76	0.28	1.89
1000	137.86	263.40	352.14	0.28	1.91

Table-3: Calculated values of Shear modulus (G in GPa), Bulk modulus (K in GPa), Young's modulus (Y in GPa), Poisson's ratio (σ) and Fracture/Toughness ratio (K/G) for MgO at different temperatures

T(K)	**G**	**K**	**Y**	**σ**	**K/G**
300	131.72	163.93	311.69	0.18	1.24
400	129.06	162.00	305.94	0.19	1.26
500	126.79	160.70	301.16	0.19	1.27
600	124.22	158.87	295.62	0.19	1.28
700	121.69	157.10	290.15	0.19	1.29
800	119.12	155.07	284.50	0.19	1.30
900	116.52	153.03	278.80	0.20	1.31
1000	113.93	151.03	273.12	0.20	1.33

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