

Thermal and Transport Properties of Mafic and Ultramafic Rocks of Oman Ophiolite

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ABSTRACT: Thermal and other physical properties of rocks and minerals are of considerable significance for deriving mineralogical and compositional models of the Earth's mantle. We have determined these properties for the mafic rock such as gabbro and ultramafic rock like harzburgite of the Oman ophiolite suite by utilizing the Debye characteristic property Θ_D . Θ_D forms the basis of our present investigation and allows us to evaluate their melting temperature T_m , thermal conductivity K_L and diffusivity D . Their seismic velocities and the density data are used, a priori, to determine the Debye temperature of these rocks. Different thermoelastic and thermodynamic relations are further used to investigate the above properties as a function of temperature, T . Our analysis shows that Θ_D is temperature dependent, indicating the presence of vibrational modes other than the Debye distribution in the gabbro and harzburgite of the Oman ophiolite. Results suggest that the thermal properties such as Θ_D , T_m and specific heat capacity c_p and transport properties such as K_L , D and viscosity, η of ultramafic rock (harzburgite) are higher than those of mafic rock, indicating the influence of an olivine content in the former. Θ_D decreases with increasing temperature but increases with increasing pressure, P . Similarly, compressibilities increase for both rocks with increasing T but decrease with increasing P . The trends of variation of thermal conductivity and diffusivity with temperature and pressure are opposite. K_L and D decrease with increasing T but are found to increase with increasing P .

Keywords: Debye temperature; Melting temperature; Specific heat capacity; Thermal conductivity; Diffusivity; Ophiolite.

الخواص الحرارية والانتقالية للصخور القاعدية وفوق القاعدية من الأفيولات العمانية

سيد العارفين و رام سنج

الملخص: الخواص الحرارية والفيزيائية للصخور والمعادن لها أهمية واضحة في استنباط النماذج المعدنية والتركيبية للقشرة الأرضية. لقد استخرجنا بعض الخواص للصخور القاعدية مثل القابرو والصخور فوق القاعدية مثل الهارزبورجيت في الأفيولات العمانية وذلك باستخدام الخواص التركيبية لدرجة حرارة ديباي Θ . درجة حرارة ديباي Θ باستخدامها كأساس في هذا البحث ساعدت في إيجاد درجة حرارة الانصهار درجة الحرارة التوصيلية K_L وكذلك عامل الانتشارية D . لقد استنبطت درجة حرارة ديباي Θ_D من قيمة سرعات الزلازل والكثافة. كذلك استخدمت الاختلافات في علاقات الحرارة البيناميكية و الحرارة الاستطالية في استنتاجات الخواص اعلاه بدلالة درجة الحرارة. أثبتت تحاليلنا أن درجة حرارة ديباي Θ_D تعتمد على درجات الحرارة مما يعزو إلي وجود حالة اهتزازية خلاف توزيع ديباي في كل من القابرو و الهارزبورجيت في الأفيولات العمانية. أوضحت النتائج أن كل من Θ_D و T_m و سعة الحرارة النوعية C_p وكذلك الخواص الانتقالية K_L و D و عامل اللزوجة η في الصخور فوق القاعدية اعلى من ذلك في الصخور القاعدية مما يدل على تأثير معدن الأولفين في الصخور فوق القاعدية. تتناقص درجة حرارة ديباي Θ_D بازدياد درجة الحرارة T ولكنها تزداد بزيادة الضغط P و K_L و D يتناقصان بازدياد درجة الحرارة T ولكنهما يتزايدان بزيادة الضغط P .

الكلمات المفتاحية: درجة حرارة ديباي Θ ، درجة حرارة الانصهار، سعة الحرارة النوعية، درجة الحرارة التوصيلية، الأفيولات.

1. Introduction

Our present understanding of the deep interior of the earth in terms of a thin crust, a mantle, a liquid outer core and a solid inner core is largely based on seismological data recorded at the network of seismic stations distributed all over the globe. However, thermal properties along with geochemical data have become increasingly important lately in the understanding of the interior of the Earth. They are of considerable significance for deriving the mineralogical and compositional models of the Earth's mantle. At depth levels of less than 700 km, thermophysical properties can help determine the tectonic and petrogenic processes involved in the generation of oceanic lithosphere. Besides providing information on the interior of the Earth, thermoelastic properties can enhance our knowledge about

the formation and transformation of rocks and minerals. The rate of deformation increases strongly with temperature but decreases with pressure at modest pressures. Thermal and transport properties of planetary materials as functions of temperature and pressure are the key to the understanding of the dynamics and evolution of terrestrial planets.

In recent years, a good deal of interest has been shown in the literature [1-6] in the study of the thermal properties of the mantle and the core. The Debye temperature, Θ_D , is one of the important ingredients in geophysical studies and has facilitated the characterization of rocks, minerals, and even geological processes such as metamorphism [7]. Any change in the external condition of rocks, and other material formation and transformation, can lead to a change in Θ_D . The Debye temperature is a physical constant of matter that characterizes numerous properties of solids, such as specific heat, electric conductivity, thermal conductivity, broadening of X-ray spectral lines, and elastic properties. In Debye theory, Θ_D , is the temperature of a crystal's highest normal mode of vibration, i.e. the highest temperature that can be achieved due to a single normal vibration. The concept was first introduced by Peter Debye in his theory of specific heat. The Debye temperature is defined by the equation, $\Theta_D = hv_D/k$, where k is Boltzmann's constant, h is Planck's constant, and ν_D is the maximum frequency of the vibrations of the atoms of a solid. It gives a relative idea for a temperature scale, above which vibrations within a solid behave basically according to the Dulong-Petit law and the heat capacity is given by $3R$, R being the gas constant. Below the Debye temperature quantum effects are important, and the heat capacity is reduced considerably at low temperatures. At $T \ll \Theta_D$, the specific heat is proportional to $(T/\Theta_D)^3$ (the Debye T^3 approximation).

The difference between the Debye temperatures of the separated facies of the metamorphic rocks is maximum in the case of regional metamorphism, is lower at an intermediate level of metamorphism, and is a minimum in the case of extremely altered rocks. Similarly, melting temperature and its pressure dependence, $T_m(P)$, are important items of information required for the thermal characterization of materials, including minerals and rocks. On the other hand, the dependence of thermal and transport properties on temperature and pressure is important information on the physical properties of rocks for understanding the driving forces in geodynamics.

In the present work we have used the seismic velocity and the density data [8, 9] to obtain useful properties such as Debye temperature, melting temperature, compressibilities, specific heat capacities, Gruneisen parameter, viscosity, thermal conductivity and diffusivity of harzburgite and gabbro by making use of thermoelastic and thermodynamic equations. Gabbro and harzburgite rock (a type of peridotite rock) of the Oman ophiolite are of considerable interest to geophysicists and geologists. The available measured density and seismic velocities of these rocks, which are the basic input of the present analysis, are uniform and consistent.

A brief description of the relevant rocks of the Oman ophiolite is given in section 2. Section 3 discusses the basic formalism for determining the temperature dependence of Debye temperature, specific heats, compressibilities and diffusivity. The melting criterion and viscosity are discussed in section 4. Section 5 describes the pressure dependence of thermal properties, and is followed by a summary and conclusion in Section 6.

2. Oman Ophiolite

Ophiolite is an integral part of many mountain belts. Study of ophiolites aids in understanding the formation of mountains and the history of sea-floor spreading [10,11] in past ocean basins. The Samail ophiolite in southeastern Oman (see Figures 1 and 2 [12, 13]) provides the best opportunity [14] to investigate the oceanic lithosphere exposed on land. From base to top, the Oman ophiolite sequence is made up of peridotite, layered gabbro, massive gabbro, dikes and volcanic rocks. The entire sequence is about 13 km thick. Harzburgite forms the bottom-most rock of the Oman ophiolite, which is a sequence of rocks representing oceanic crustal and upper mantle material that has been pushed up onto the continents. Olivine is the major constituent mineral of the upper mantle, with an average composition of 90% mol Mg_2SiO_4 and 10% mol Fe_2SiO_4 [10]. About 80% of the harzburgite of the Oman ophiolite suite is olivine. The thermoelastic properties of harzburgite will, therefore, provide us with a better understanding of the composition and dynamics of the upper mantle. Harzburgite is a type of peridotite rock, abundantly found in the upper mantle and predominantly composed of the minerals olivine and orthopyroxene, and relatively low proportions of basaltic ingredients. It has a uniform mineralogy of 80% olivine ($(Fe, Mg)_2SiO_4$), 17–19% orthopyroxene ($(Mg, Fe)_2Si_2O_6$), 1% chrome spinel ($(Mg, Fe)(Al, Cr)_2O_4$) and 1% clinopyroxene ($(Ca, Mg, Fe, Al)_2(Si, Al)_2O_6$).

Gabbro, an igneous rock, is another major constituent of the Oman ophiolite suite. The gabbroic layer is interlayered between the mantle peridotite and the sheeted dyke complex. It represents the crustal succession of the Oman ophiolite with a thickness ranging from about 1.5 km to 4 km. It is believed to have been generated in a magma chamber beneath an ancient fast-spreading ocean ridge. The largest part of the gabbroic layer is composed of troctolite, olivine gabbro and gabbro with minor wehrlite and dunite. Gabbro is mainly composed of calcium plagioclase, pyroxene and olivine minerals. The percentage of olivine present in the gabbro of the Oman ophiolite ranges from 18% to 44% [15].

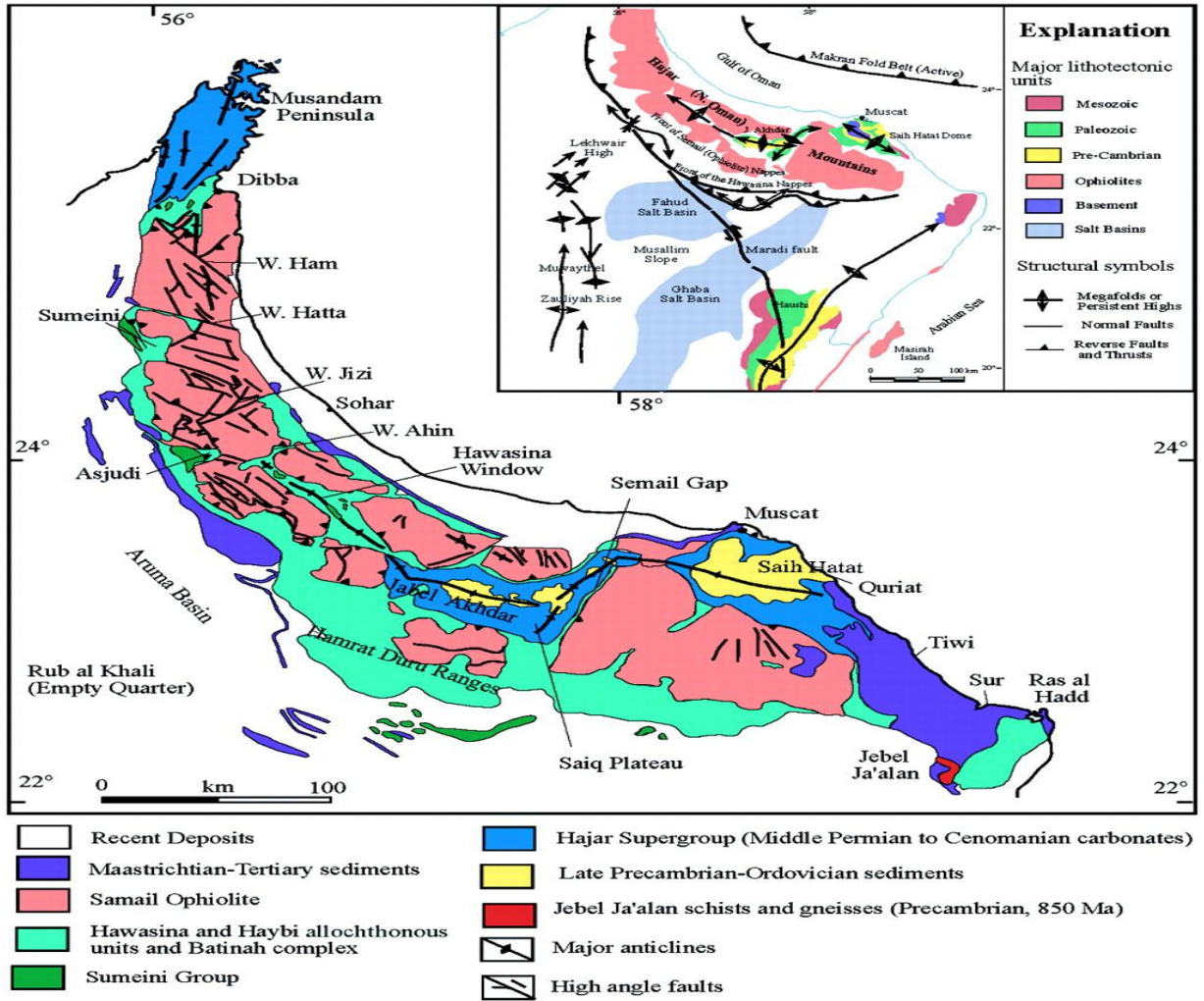


Figure 1. Geology of Oman showing Semail ophiolite in pink [12]

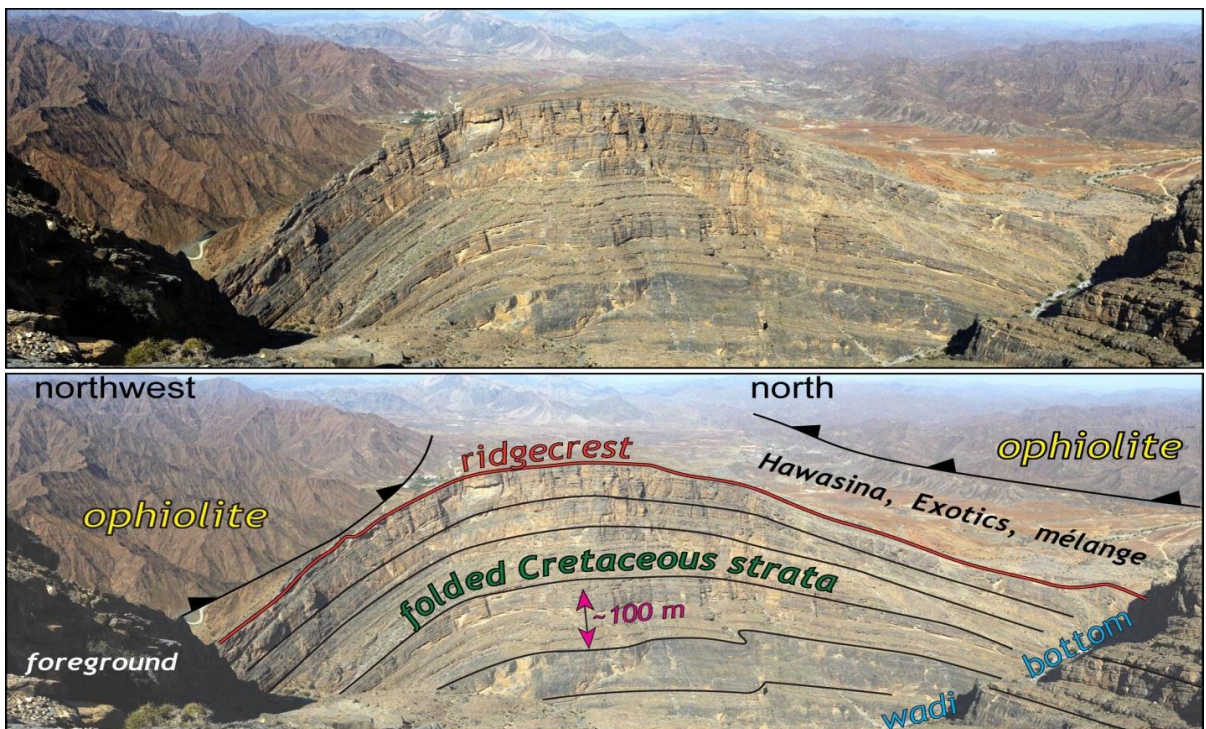


Figure 2. Exposed rocks of the Oman ophiolite and its associates [13]

3. Temperature Dependence of Thermophysical Properties

3.1 Debye Temperature

The Debye theory connects the heat capacity of a poly-atomic solid with its elastic constants, and paves the way for calculating the characteristic temperature from the measured data of density and velocities of primary (p-wave) and secondary or shear (s-wave) ultrasonic waves in the solid. Here we have used acoustical data [8] to obtain Debye temperature. In terms of acoustic velocities, Θ_D , also known as acoustic Debye temperature in geophysical literature, takes the simplified form [16]:

$$\Theta_D(T) = 251.2 \left(\frac{\rho(T)}{\mu(T)} \right)^{1/2} v_m(T) \quad (1)$$

ρ is the density (g cm^{-3}) and μ is the mean atomic mass given by M/p ; M is the molecular weight (g mol^{-1}) and p is the atomic number. For composite materials like harzburgite and gabbro, the mean atomic mass, μ is taken as 21 g mol^{-1} [17]. v_m is the generalized mean velocity (km s^{-1}) given by:

$$v_m(T) = \left[\frac{1}{3} (v_p^{-3}(T) + 2v_s^{-3}(T)) \right]^{-1/3} \quad (2)$$

where v_p and v_s are the acoustic velocities of the primary (longitudinal) and secondary (transverse) waves. We have used experimentally determined values of v_p , v_s , ρ and an empirical value of mean atomic mass 21 amu in Eqs. (1) and (2) to calculate Θ_D [8, 9].

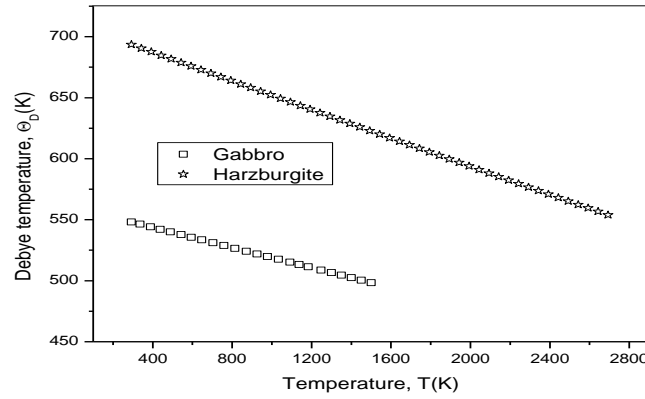


Figure 3: Variation of Debye temperature (Θ_D) of gabbro and harzburgite with temperature

We have calculated the temperature dependence of density and velocity of the mafic and ultramafic rocks from the available data [8, 9]. The values of Θ_D obtained at different temperatures of gabbro and harzburgite are plotted in Figure 3, which shows that Θ_D decreases linearly with increasing temperature of the rock. Typical values of Θ_D at room temperature (293.15K) for gabbro and harzburgite are found to be 548 K and 693K. Θ_D for harzburgite is about 26% higher than that of gabbro. The higher value for harzburgite may be due to the abundance of olivine in it. There are hardly any data on Θ_D of these rocks available in the literature. It may be recalled that gabbro and harzburgite are composed of 40% and 80% olivine respectively. Θ_D for olivine is found to be 731 K [18]. In view of this, the computed Θ_D for gabbro and harzburgite are well within the expected range.

3.2 Specific Heat as a Function of Temperature

The Debye theory was originally developed for monatomic solids for which the vibrational phonon density of states is given by Debye frequency spectrum. The theory can be applied to polyatomic solids like rocks and minerals provided the density of states can be approximated by the frequency spectrum [19]. Taking into account all the possible modes of acoustic vibrations, the total phonon energy, U_D becomes [19]:

$$U_D = 9Nk_B T \left(\frac{T}{\Theta_D} \right)^3 \int_0^{x_D} \frac{x^3 dx}{(e^x - 1)} \quad (3)$$

The upper limit of integration, x_D refers to:

$$x_D = \frac{h\omega_D}{2\pi k_B T} \quad (4)$$

where h is the Planck's constant, ω_D is the Debye angular frequency and k_B is the Boltzmann's constant. Differentiating Eq. (3) with respect to T , one obtains specific heat at constant volume:

$$c_V = 9Nk_B \left(\frac{T}{\Theta_D} \right)^3 \int_0^{x_D} \frac{x^4 e^x dx}{(e^x - 1)^2} \quad (5)$$

The integral has been evaluated here numerically by using the value of Θ_D (=548 K) as determined in section 3.1. A plot of c_V against the ratio, T/Θ_D is shown in Figure 4. The curve approaches the maximum value of $25 \text{ J mol}^{-1} \text{ K}^{-1}$ at higher temperatures, which is the highest limiting value of $3R$ (R being the gas constant) due to Dulong Petit's law. At low temperature ($T < \Theta_D$), C_V increases with increasing temperature as per Debye's T^3 law.

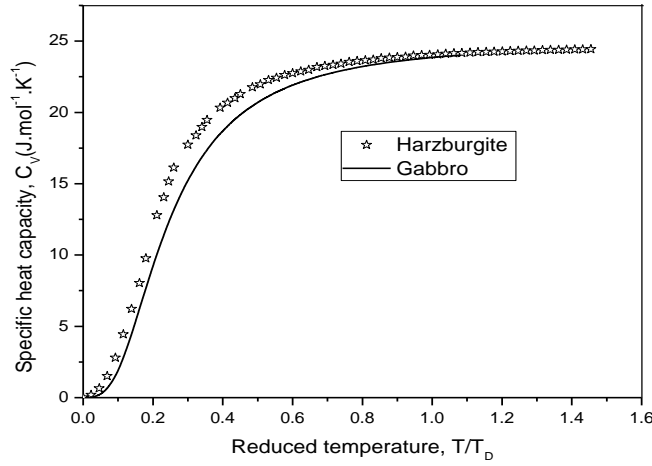


Figure 4. The computed values of the Debye specific heat (c_V) of gabbro and harzbutgite plotted against T/Θ_D

3.3 Compressibilities

3.3.1 Isothermal and Adiabatic Compressibilities

Specific heat capacities are related to isothermal compressibility, κ_T and the coefficient of volume expansion, β through a thermodynamic relation:

$$c_P = c_V + \frac{TV\beta}{\kappa_T} \quad (6)$$

Specific heats and compressibilities are also related as:

$$\gamma = \frac{c_P}{c_V} = \frac{\kappa_T}{\kappa_S} \quad (7)$$

where κ_S is the isentropic compressibility. From Eqs. (6) and (7) one has:

$$\gamma = 1 + \frac{TV\beta^2}{c_P \kappa_S} \quad (8)$$

κ_S and κ_T minerals have been determined here from acoustic data. The adiabatic compressibility κ_S is determined [20] from the measured values of density (ρ), and longitudinal (v_l) and transverse (v_t) velocities by using the relation:

$$\kappa_S(T) = \frac{1}{\rho(T) \left[v_l^2(T) - \frac{4}{3} v_t^2(T) \right]} \quad (9)$$

Further, the isothermal compressibility, κ_T is related to Poisson ratio σ , density ρ and p-wave velocity v_p by the equation:

$$\kappa_T(T) = \frac{3[1-\sigma(T)]}{[1+\sigma(T)] \rho v_p^2} \quad (10)$$

where σ is expressed in terms of the two velocities by the equation:

$$\sigma(T) = \frac{[v_l^2(T) - 2v_t^2(T)]}{2[v_l^2(T) - v_t^2(T)]} \quad (11)$$

The computed values of κ_S and κ_T for gabbro and harzburgite are plotted in Figures 5 and 6, respectively, as functions of temperature. κ_S and κ_T are found to increase with increasing temperature. κ_T is slightly higher than κ_S . At room temperature the difference between κ_S and κ_T is small, but the difference increases with increasing temperature. γ is determined using the values of κ_S and κ_T in Eq. (7). It is found to be 1.009296 and exhibits very

little dependence on temperature. The results given in Figures 5 and 6 suggest that κ_S and κ_T of gabbro are higher than those of harzburgite. At ambient condition, κ_S of gabbro is 36% higher than that of harzburgite.

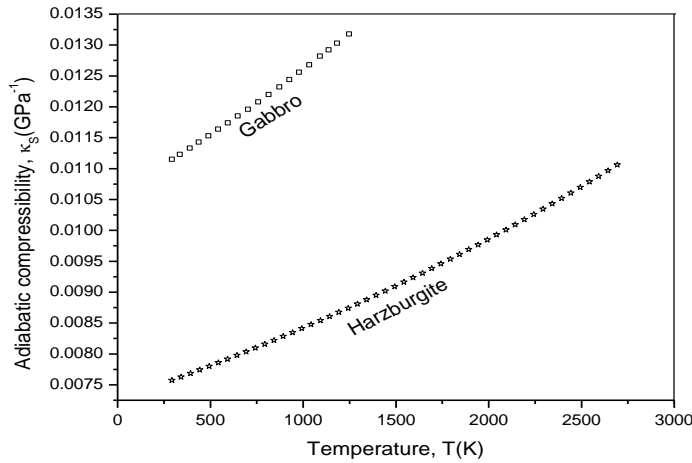


Figure 5. Comparison of of temperature dependent adiabatic (κ_S) compressibility of gabbro and harzburgite

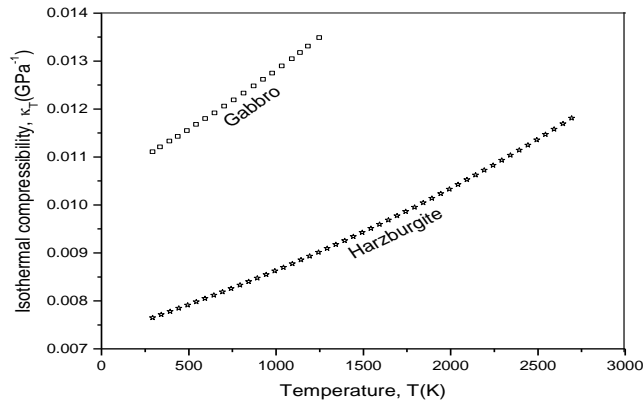


Figure 6. Comparison of of temperature dependent isothermal (κ_T) compressibility of gabbro and harzburgite

3.3.2 Specific Heat at Constant Pressure from Thermodynamic Relations

It may be noted that γ for most solid rocks is very close to unity. γ is used in Eq. 8 to determine c_p . The thermodynamic values of c_p for mafic rock (gabbro) and ultramafic rock (harzburgite) are calculated as 678.1 and 795.7 J kg⁻¹ K⁻¹ respectively at room temperature of 293.15 K. This yields the specific heat at constant volume, c_v as 671.0 J kg⁻¹ K⁻¹ for gabbro and 787.5 J kg⁻¹ K⁻¹ for harzburgite. These values are in very good agreement with the measured values [21] of 650 J.kg⁻¹.K⁻¹ for gabbro and 771 J kg⁻¹ K⁻¹ for harzburgite. In the case of gabbro a variation in specific heat capacity value of 650-1000 J kg⁻¹ K⁻¹ is reported [21]. By using the value of mean atomic mass of 21.0 amu, c_p and c_v reduce to 14.24 and 14.1 J mol⁻¹ K⁻¹ for gabbro and 16.71 and 16.54 J mol⁻¹ K⁻¹ for harzburgite respectively. We may recall that, from Debye theory, c_v at room temperature has been computed to be 21.1 for mafic and 19.1 J.mol⁻¹.K⁻¹ for ultramafic rocks, figures which are about 50% and 15.5% higher than the thermodynamic values. The difference increases at higher temperatures. It was argued [17] that the similarity between heat capacities obtained thermodynamically and from Debye theory can be used as a criterion for a material to be classified as a Debye-like solid. We can see that the two values are far from being close to each other, indicating that the mafic and ultramafic rocks of Oman ophiolite are not Debye-like solids.

3.4 Thermal Conductivity

From the striking linearity of a plot of Θ_D against K_L for silicate minerals, an empirical relation has been proposed by Horai and Simmons [22] connecting the two as:

$$K_L(T) = 0.0164\Theta_D(T) - 6.292 \quad (12)$$

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where K_L is measured in $\text{W m}^{-1} \text{K}^{-1}$ and Θ_D in K . Although the above equation was proposed for silicate minerals, the effect of chemical composition was taken into consideration in establishing Eq. (12), and hence, it has been suggested [22] that it can be applied to a wide range of materials. Equation (12) can be used for evaluating K_L , provided Θ_D is known. The thermal conductivity for gabbro determined from Eq. (12) is found to be $2.68 \text{ W m}^{-1} \text{K}^{-1}$, which compares well with the measured value of $2.47 \text{ W m}^{-1} \text{K}^{-1}$ [23], while it is $5.07 \text{ W m}^{-1} \text{K}^{-1}$ for harzburgite which is higher than the value $2.69 \text{ W m}^{-1} \text{K}^{-1}$ reported in [23]. Rocks of similar genesis may have quite different thermophysical properties because of their origin from different geological provinces and their different ages [24].

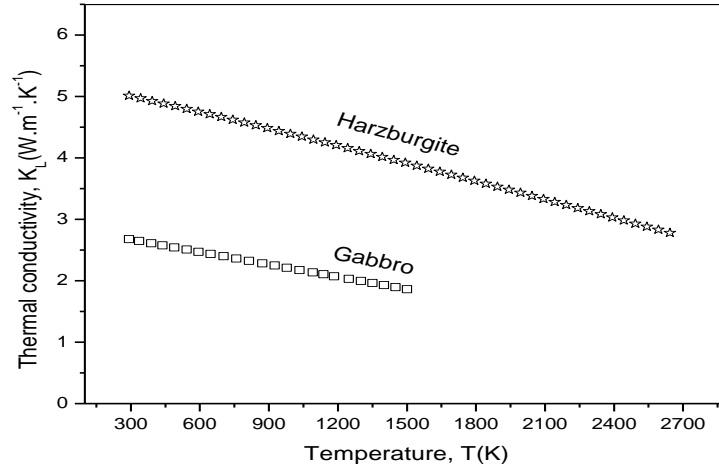


Figure 7. Dependence of thermal conductivities of gabbro and harzburgite on temperature

According to Wiedemann-Franz law the ratio of the thermal conductivity, K_L to the electrical conductivity, σ is given by:

$$\frac{K_L}{\sigma} = LT \quad (13)$$

where σ is the electrical conductivity and $L = 2.45 \times 10^{-8} \text{ W } \Omega \text{ K}^{-2}$ is the Lorentz constant. This yields the electrical conductivity for gabbro, $\sigma_{gabbro} = 3.619 \times 10^5 \text{ SI m}^{-1}$ and for harzburgite, $\sigma_{harzburgite} = 6.186 \times 10^5 \text{ SI m}^{-1}$ at normal temperature 300 K. Our results of K_L and σ suggest that harzburgite is a better conductor for heat and electricity than gabbro.

3.5 Thermal Diffusivity and Activation Energy

In the heat transfer analysis, thermal diffusivity, D plays an important role which measures the ability of a material to conduct thermal energy relative to its ability to store thermal energy. It is defined as the ratio of the thermal conductivity, K_L to the product of the density, ρ and the specific heat capacity, c_p , i.e.:

$$D(T) = \frac{K_L(T)}{\rho(T)c_p(T)} \quad (14)$$

where K_L is the lattice thermal conductivity, c_p is the specific heat capacity at constant pressure, and ρ is the density. The magnitude of thermal diffusivity dictates how fast heat moves through a material. We have used our determined values of $K_L(T)$, $c_p(T)$ and $\rho(T)$ to determine temperature dependence of the diffusivity. The thermal diffusivity value of the ultramafic rock (harzburgite) determined in this study is $2.15 \text{ mm}^2 \text{ s}^{-1}$ which is close to the measured value of peridotite (also a an ultramafic rock and similar to harzburgite in composition) from Oman ophiolite is $2.27 \text{ mm}^2 \text{ s}^{-1}$ [24]. The thermal diffusivity value of $1.3 \text{ mm}^2 \text{ s}^{-1}$ determined here for the mafic rock (gabbro) is slightly higher than the experimental value of $0.97 \text{ mm}^2 \text{ s}^{-1}$ [21]. $D(T)$ of both mafic and ultramafic rocks fall with increasing temperature. The decrease in $D(T)$ for ultramafic rock is much sharper that of gabbro in the lower range of temperature. At high T , $D(T)$ tends towards a constant value.

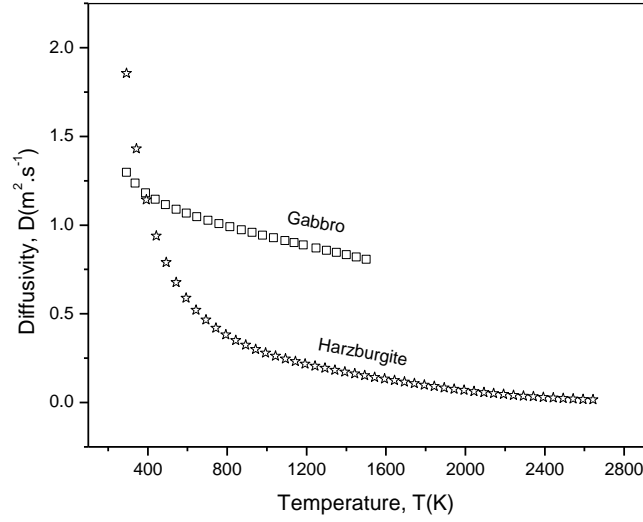


Figure 8. Dependence of diffusivities of gabbro and harzburgite on temperature

The formation of mafic and ultramafic rocks at the deep interior of the Earth involves complex chemical reactions and phase changes under the influence of high temperature and pressure. The activation energy ΔE is a measure of the energy necessary for a chemical reaction to occur. The repulsive energy emerging due to the overlap of electron clouds needs to be overcome by the activation energy. The computed values of $D(T)$ have been fitted to an Arrhenius type equation,

$$D = D_0 e^{-\Delta E/RT} \quad (15)$$

where R is the gas constant. Taking the natural logarithm, one has:

$$\ln D = \ln D_0 + \left(-\frac{\Delta E}{R}\right) \frac{1}{T} \quad (16)$$

The plot of $\ln D$ vs $1/T$ results in a linear variation. The slope has been used to determine ΔE . For gabbro ΔE is found to be 1.4 kJ which is much lower than that (4.3 kJ) of harzburgite.

4. Melting Temperature and Viscosity

4.1 Melting Criterion

We suggest a simple approach to determine the melting temperature from the knowledge of the Debye temperature, Θ_D , which we obtained in section 3.1. Lindemann [25] proposed that the amplitude of the atomic vibrations increase with increasing temperature and that melting occurs when the amplitude of vibrations reach a critical fraction, y_m of the mean atomic radius, R_a . Mott and Jones [20] used the Debye model to show that the mean square amplitude of vibration of each atom is given by $\left(\frac{3h}{2\pi\Theta_D}\right)^2 \left(\frac{T}{Mk_B}\right)^{1/2}$ approximately. Using this expression, Lindemann's formula can be written [26]:

$$T_m = \left(\frac{2\pi}{3h} y_m R_m \Theta_D\right)^2 M k_B \quad (17)$$

where y_m is the maximum amplitude of vibration [27] which is taken as 0.2. Θ_D is the Debye temperature (K), R_m the mean atomic radius and M the mean atomic mass. The value of M is taken 21 amu for gabbro and harzburgite. k_B is the Boltzmann's constant and h is the Planck's constant. The mean atomic radius is calculated from the relation:

$$R_m = \left(\frac{3M}{4\pi\rho}\right)^{1/3} \quad (18)$$

The melting temperature of gabbro and harzburgite calculated from the above relations are 1201 K and 1695 K, which are much higher than the corresponding Debye temperatures, 548 K and 693 K. T_m is, in general, sensitive to the values of R_m , Θ_D and y_m as can be seen from Eq. (17).

4.2 Viscosity

The viscosity, η_m of gabbro and harzburgite at their melting points can be determined [27, 28] from the values of M , T_m and V_m i.e.

$$\eta_m = 1.6 \times 10^{-4} \frac{\{MT_m\}^{1/2}}{V_m^{2/3}} \quad (19)$$

where viscosity, η_m is given in mPa s. V_m is the atomic volume at melting and M is the molecular weight. Equation (19) is found to reproduce the experimental viscosity data for liquid metals at their melting points with great success. We have collected the values, Θ_D , T_m , c_V , K_L , D and η determined in this work at normal T and P in Table 1. The viscosity values for the melting phase of gabbro and harzburgite determined from Eq. (19) are found to be 2.21 mPa s and 2.63 mPa s. at their corresponding melting points (1201 K and 1695 K) respectively. It may be noted that all the values of thermal properties of harzburgite are larger than those of gabbro except for thermal conductivity.

Table 1. Debye temperature Θ_D (K), melting temperature T_m (K), specific heat capacity c_P (J kg⁻¹ K⁻¹), thermal conductivity K_L (W m⁻¹ K⁻¹), diffusivity D (mm² s⁻¹) and viscosity η (mPa s) of gabbro and harzburgite; published values for each rock are shown in bracket.

Properties Rocks	Θ_D (K)	T_m (K)	c_P (J kg ⁻¹ K ⁻¹)	K_L (W m ⁻¹ K ⁻¹)	D (mm ² s ⁻¹)	η (mPa s)
Gabbro	548	1201 1123 ^[9]	678.0 650.0 ^[21]	2.66 2.47 ^[21]	1.30 0.97 ^[21]	0.00221
Harzburgite	693 731 ^{[18]**}	1693 2163*,1473 [§]	796.0 771 ^[21]	5.07 2.69 ^[21]	1.8 2.27 ^[24]	0.00263

*Melting temperature of Mg_2SiO_4 ; §Melting temperature of Fe_2SiO_4 . It may be noted that for our model Mg_2SiO_4 constitutes 90% of olivine, which is about 80% of Oman harzburgite. Fe_2SiO_4 constitutes about 10% of olivine.

** Debye temperature of olivine

5. Pressure Dependence of Thermal Properties of Gabbro

The pressure dependence of Debye temperature, specific heat capacity, adiabatic compressibility, isothermal compressibility, thermal conductivity, and diffusivity can be determined from the various equations developed in the previous sections, provided that the pressure dependence data for density and seismic velocities are known. The basic input data (seismic velocities) available for gabbro are taken from reference [8]. The sample of gabbro for which these measurements exist was taken from a depth of 5.5 km. There are no pressure dependent velocity data available for harzburgite in the literature. In this section, we have therefore restricted our discussions of pressure dependent properties to those of gabbro only.

5.1 Pressure Dependence of Density and Velocity

The pressure dependence of the densities of gabbro and harzburgite are determined using the Murnaghan equation [29]:

$$\rho(P) = \rho_0 \left[1 + \frac{b_1 P}{3B_0} \right]^{1/n} \quad (20)$$

where ρ_0 is the density at atmospheric pressure, B_0 the bulk modulus, b_1 the pressure gradient of B_0 and P the pressure. The pressure dependent density and velocity data of gabbro are plotted in Figs. 9 and 10. The density data show a linear relationship but the velocity data show a non-linear relationship with pressure.

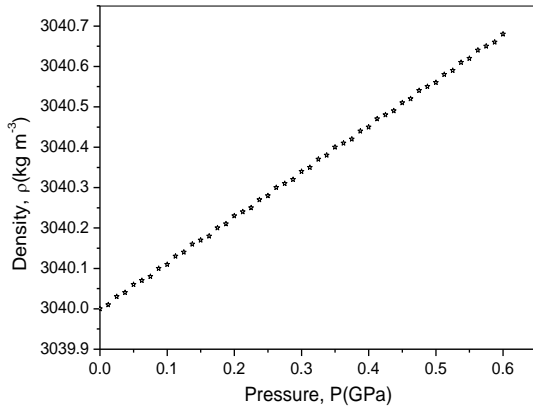


Figure 9. Plot of density of gabbro as a function of pressure

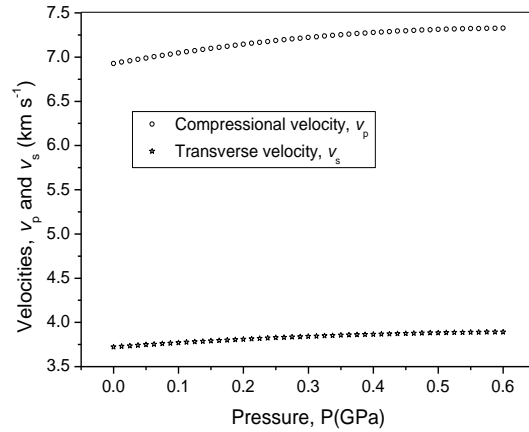


Figure 10. Variation of longitudinal and transverse wave velocity of gabbro with pressure

5.2 Numerical Results for Debye Temperature, Compressibilities, Specific Heat Capacity, Thermal Conductivity and Diffusivity as a Function of Pressure

The pressure dependence of Debye temperature, specific heat capacity, compressibilities, thermal conductivity, and diffusivity are plotted in Figures 11-15. The value of Θ_D of gabbro increases from its value of 548 K at ambient temperature and pressure to a value of 574 K at 0.60 GPa. It can be seen from Figure 11 that Θ_D increases with increasing P but does not exhibit a linear variation like Θ_D - T variation as found in Figure 3. At high pressures, the gradient $d\Theta_D/dP$ is much smaller than that at low pressures. It is expected to be lower at higher pressures because various vibrational modes are likely to be compressed resulting in a lower gradient of $d\Theta_D/dP$.

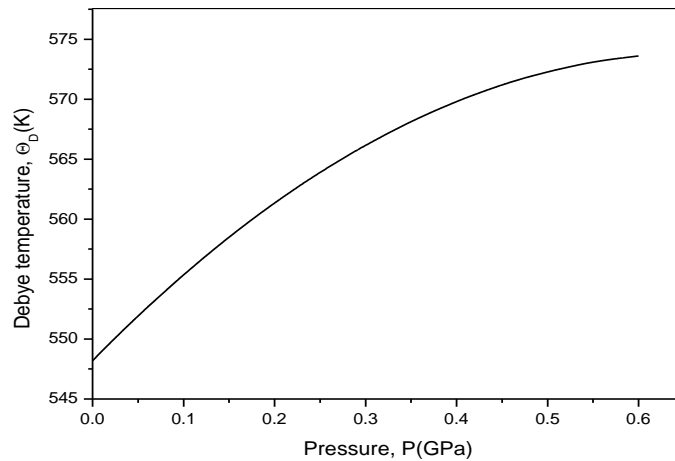


Figure 11. Variation of Debye temperature (Θ_D) of gabbro with pressure.

The pressure dependence of specific heat capacity, c_V , is shown in Figure 12. It is determined from Eq. (5) using the values of $\Theta_D(P)$ as shown in Figure 11. With increasing pressure, c_V decreases nonlinearly from its value of $21.1 \text{ J mol}^{-1} \text{ K}^{-1}$ at ambient pressure to about $19.6 \text{ J mol}^{-1} \text{ K}^{-1}$ at a pressure of 0.6 GPa. This amounts to a decrease of c_V by 7.5%.

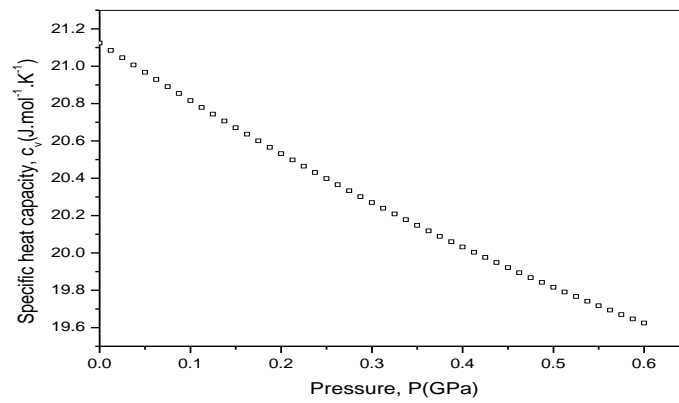


Figure 12. Variation of specific heat capacity, c_V , of gabbro as a function of pressure.

The computed values of κ_S and κ_T are plotted in Figure 13 as a function of P . κ_S is approximately equal to κ_T at ambient conditions but the difference between them increases as P increases. κ_S is smaller than κ_T at high P which suggests that the specific heat ratio, γ , slowly increases with increasing pressure.

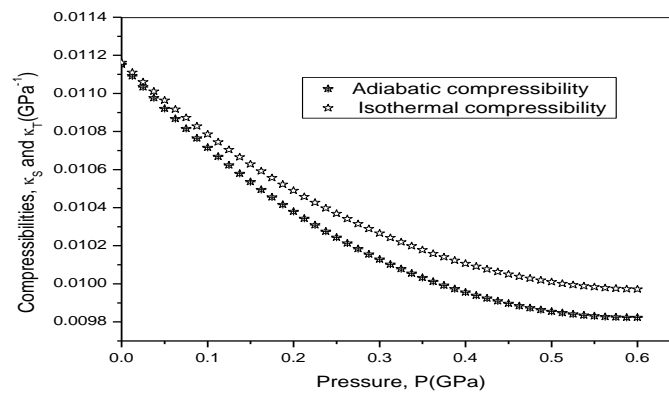


Figure 13. Adiabatic and isothermal compressibilities of gabbro shown as a function of pressure.

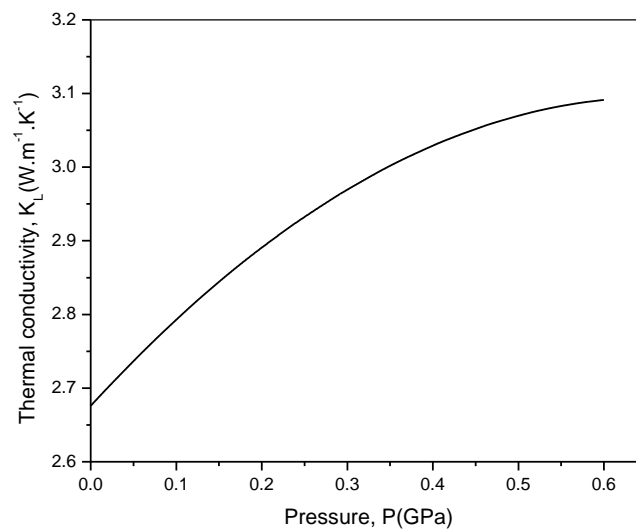


Figure 14. Variation of thermal conductivity, K_L of gabbro as a function of pressure.

The thermal conductivity K_L and diffusivity D of gabbro as a function of pressure are plotted in Figures 14 and 15. Both K_L and D increase with increasing P . Like $d\Theta_D/dP$, the gradients dK_L/dP and dD/dP are large at lower pressures and decrease as P increases. K_L and D increase by 10% and 61% respectively as P increases to 0.6 GPa from 0 GPa.

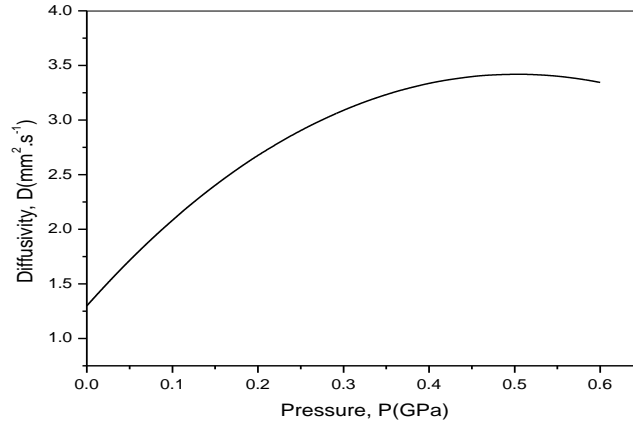


Figure 15. Diffusivity, D of gabbro as a function of pressure.

6. Conclusion

The seismic velocities and the density data are used to determine the temperature dependence of Debye temperature, (Θ_D) and other thermodynamic and thermoelastic functions, such as specific heat capacity (c_p and c_v), compressibilities (κ_S and κ_T), thermal conductivity (K_L), and the diffusivity (D) of gabbro and harzburgite. Θ_D as determined here, was further used to compute the melting temperature T_m and the viscosity (η). The availability of experimental data for the seismic wave velocities [25] for gabbro over a wide pressure range of 0 to 6 kbar has made it possible to also compute the pressure dependence of Θ_D , c_v , κ_S , K_L and D of gabbro.

Θ_D computed at ambient conditions for gabbro is 548 K and for harzburgite is 693 K. Θ_D for harzburgite is about 26% higher than that of gabbro. Θ_D for both rocks falls linearly with increasing temperature. The specific heat ratio (γ) for gabbro and harzburgite at normal P and T are found to be around 1.009 and 1.0103 respectively. This value of γ is consistent with the observation [21] that γ is nearly unity for rocks and minerals. γ is found to depend weakly on T .

The value of γ has been utilized to calculate the specific heat capacities, c_p and c_v , through thermodynamic relations. The values of c_p and c_v for gabbro are found to be 14.33 J mol⁻¹ K⁻¹ and 14.20 J mol⁻¹ K⁻¹ respectively at room temperature, 293.15 K. Additionally, we have estimated c_v from Debye theory where Θ_D occurs as an input. The value of c_v at room temperature is obtained as 21.12 J mol⁻¹ K⁻¹ and the c_p as 21.31 J mol⁻¹ K⁻¹. It may be noted that c_p and c_v of gabbro determined from thermodynamic relation is about 33% lower than that determined from Debye theory. c_p and c_v values for harzburgite determined from thermodynamic relation are 16.71 J mol⁻¹ K⁻¹ and 16.54 J mol⁻¹ K⁻¹ and those determined from Debye theory are 19.31 J mol⁻¹ K⁻¹ and 19.11 J mol⁻¹ K⁻¹ respectively. In this case, specific heat capacity determined from thermodynamic relations is 13% lower than that computed from Debye theory. Specific heat capacities are found to increase with increasing temperature. The crucial criterion for determining [2] whether or not a polyatomic solid is a Debye-like solid is the closeness between the thermodynamic value of c_v and its value calculated from Debye theory. These values exhibit little or no closeness indicating that the gabbro and harzburgite of the Oman ophiolite suite are not Debye-like solids.

Melting point has been calculated from modified Lindemann's formula by making use of Debye temperature as input. T_m of harzburgite at ambient conditions is found to be 1693 K compared to 1201 K for gabbro. It may be noted that T_m for harzburgite is about 40% higher than that of gabbro. The computed value of viscosity of molten gabbro (0.00221 mPa s) is smaller than that of the molten harzburgite (0.00263 mPa s) by about 16%. We may recall that Mg, Fe and Si are the main constituent elements of these rocks. It is interesting to observe that the viscosities of these rocks fall within the range of the experimental values [30] of viscosity of Mg (1.25 mPa s), Fe (5.5 mPa s) and Si (0.94 mPa s).

The pressure dependence of Θ_D , c_v , κ_S , κ_T , K_L and D for gabbro have been computed as a function of pressure. This was possible by virtue of available experimental seismic velocity data for gabbro. The computed value of Θ_D , K_L and D are found to increase with increasing P , unlike their temperature dependence. However, specific heat (c_v) and compressibilities (κ_S and κ_T) of gabbro decrease with increasing pressure. Θ_D , T_m , η , c_v , κ_S , κ_T , and D are smaller in mafic rocks (gabbro) than those of ultramafic rocks (harzburgite) except for the thermal conductivity, K_L . This behavior indicates the influence of the olivine content (80% in harzburgite and up to 40% in gabbro) on the thermal and transport properties of these rocks. The higher thermal conductivity of gabbro is likely to cause its solidification faster than is the case for harzburgite.

References

1. Anderson, O.L. Thermoelastic properties of MgSiO₃ perovskite using Debye approach, *American Mineralogist*, 1998, **83**, 23-35.
2. Anderson, O.L., Isaak D.G. and Nelson, V.E. The high-pressure melting temperature of hexagonal close-packed iron determined from thermal physics, *J. Phys. and Chem. Solids*, 2003, **64**, 2125-2131.
3. Anderson, D.L. Temperature and pressure derivatives, *J. Geophys. Res.*, 1988, **93**, 4688-4700.
4. Sternik, M. and Parlinski, K. Ab initio calculations of the stability and lattice dynamics of the post-perovskite, *J. Phys. Chem. Solids*, 2006, **67**, 796-800.
5. Fujiwara, H., Ueda, Y., Awasthi, A., Krishnamurthy, N. and Garg, S.P. Thermodynamic study on refractory metal silicides, *J. Phys. Chem. Solids*, 2005, **66**, 298-302.
6. Wei Lu and Baosheng Li, Thermal equation of state of (Mg_{0.9}Fe_{0.1})SiO₄ olivine, *Phys. Earth. Planet. Inter.*, 2006, **157**, 188-195.
7. Dergachov, A. L. and Starostin, V.I. The Debye characteristic temperature as indicator for formation and transformation conditions of rocks and ores, *Ore Deposit Geology*, 1981, **6**, 67-75.
8. Christensen, N.I. and Smewing, J.D. Geology and seismic structure of the northern section of the Oman ophiolite, *J. Geophys. Res.*, 1981, **86**, 2545-2555.
9. Liping, B., Jianguoang, D. and Wei, L. Experimental studies of electrical conductivities and P-wave velocities of gabbro at high pressures and high temperatures, *Sci. China, Ser. D Earth Sci.*, 2003, **46**, 895.
10. Moores, E.M. and Jackson, E.D. Ophiolites and oceanic crust, *Nature*, 1974, **228**, 837-842.
11. Coleman, R.G., Introduction to the Oman ophiolite special issue, *J. Geophys. Res.*, 1981, **86**, 2495-2496.
12. Kusky, T., Robinson, C. and El-Baz, F. Tertiary–Quaternary faulting and uplift in the northern Oman Hajar Mountains, *Journal of the Geological Society*, 2005, **162**, 871-888, doi:10.1144/0016-764904-122 <http://wmblogs.wm.edu/cmbail/dispatches-from-oman-juxtaposition/>
13. Boudier, F. and Coleman, R.G. Cross-section through the peridotite in the Samail ophiolite, Southeastern Oman, *J. Geophys. Res.*, 1981, **86**, 2573-2592.
14. Korenaga, J. and Klemen, P.B., Origin of gabbro sills in the Moho transition zone of the Oman ophiolite: Implications for magma transport in the oceanic lower crust, *J. Geophys. Res.*, 1997, **102**(B12), 27,729-27,749.
15. Arafin, S., Singh, R.N. and George, A.K. Extension of Lindemann's Formula to Study the Pressure Dependence of Melting Temperature *Int. J. Thermophys.* 2012, **33**:1013–1022, DOI 10.1007/s10765-012-1227-8S.
16. Anderson, O.L. Equations of State of Solids for Geophysics and Ceramic Science, Oxford University Press, New York, 1995
17. Anderson, O.L. Isaak, D.G. *Mineral Physics and Crystallography, A Handbook of Physical Constants*, AGU Reference Shelf 2, 1995, 64-97
18. Kittel, C. *Introduction to Solid State Physics*, (7th Edition), Wiley, New York, 1996.
19. Mott, N.F. and Jones, H. *The Theory of the Properties of Metals and Alloys*, (2nd Edition). Oxford University Press, Oxford, 1936.
20. Waples, D.W. and Waples, J.S. A Review and Evaluation of Specific Heat Capacities of Rocks, Minerals, and Subsurface Fluids. Part 1: Minerals and Nonporous Rocks, *Natural Resources Research*, 2004, **13**, 97-122.
21. Horai, K. and Simmons, G. An empirical relationship between thermal conductivity and Debye temperature for silicates, *J. Geophys. Res.*, 1970, **75**, 678.
22. Keiffer, H.H. Temperature of rock thermal properties, File=/xtex/tes/krc/HeatOfT.tex 2010feb, July 19, 2010
23. Mottaghy, D., Vosteen, H.D. and Schellschmidt, R. Temperature dependence of the relationship of thermal diffusivity versus thermal conductivity for crystalline rocks. *Int. J. Earth Sci*, 2008, **97**(2), 435-442. DOI 10.1007/s00531-007-0238-3.
24. Gibert, B., Seipold, U., Tommasi, A. and Mainprice, D. Thermal diffusivity of upper mantle rocks: Influence of temperature, pressure, and the deformation fabric, *J. Geophys. Res.*, 2003, 108 : 2359.
25. Lindemann, F.A. Uber die Berechnung molecularer *Eigenfrequenzen*, 1910, *Phys. Z.* 11, 609–612.
26. Faber, T.E., *Introduction to Theory of Liquid Metals*, Cambridge University Press, Cambridge, 1972.
27. Andrade E.N. A theory of the viscosity of liquids, *Phil. Mag.*, 1934, **17** : 497
28. Iida, T. and Guthrie, R.I.L. *The Physical Properties of Liquid Metals*, Clarendon Press, Oxford, 1988.
29. Anderson, D.L., *Theory of the Earth*, Caltech Books, Caltech, Pasadena, 1989.
30. Brandes, E.A. and Brook, G.B. (Edited), *Smithsells Metals Reference Book* (7th Edition), Butterworth-Heinemann, Oxford, 1992.

Received 6 December 2015

Accepted 29 February 2016