PHYSICAL PROPERTIES OF OXIDES AND SILICATES AT HIGH PRESSURES AND TEMPERATURES*

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(ABSTRACT)

Values of 14 parameters are tabulated for 56 minerals (oxides and silicates), including density, mole weights and volumes, and elastic moduli. The elasticity is found to be very much dependent on the oxygen packing density and, to a smaller extent, on the valency, electronegativity, etc., of the cations. The entropy is correlated with the volume, while the free energy is more dependent on the properties of the cations. Some of the physical and thermodynamic parameters show additivity; the summation should be made over the volumes. The density and elastic moduli of rocks and minerals are discussed as functions of temperature and pressure. The degree of variation with pressure bears a direct relation to the oxygen density.—Author's Abstract

Detailed structural studies have been made of oxides and silicates [1 - 4], and their main physical and thermodynamic parameters have been determined [5 - 8]. The density and elastic parameters have been examined over a wide range in P [5, 9 - 14], and some fragmentary results have been reported [5, 15 - 18] on the effects of T on these. Concepts from atomic physics have been used [17, 18] to derive a theory of the equations of state for these substances, but little has been published on the relation of crystal structure to physical properties for minerals; thus, many concepts from mineralogy and chemical crystallography have been inadequately used in studying the internal structure of the Earth. In particular, more attention should be given to the close-packing concept for oxygen ions in minerals, since the crust, mantle, and (in part) the outer core consist of oxides and silicates [17, 19 - 21]. Chemical crystallography provides insight into the physical basis of the changes during differentiation of the material of the Earth [20 - 22].

This paper is a continuation of a previous one [23] and gives a quantitative description of the oxygen-ion packing density in oxides and silicates, together with a consideration of the effects on some physical and thermodynamic parameters. The effects of P and T on physical properties are also considered.

OXYGEN-ION PACKING IN OXIDES AND SILICATES

First I discuss the advantages of considering together oxides and silicates as regards oxygen-anion packing. In Povarennykh's classification [4], oxides and silicates are assigned to different classes of a major type (oxygen compounds). Binary oxides and complex oxides and complex oxides of the spinel type are assigned mainly to the subclass of coordination compounds on the basis of the principal structural pattern, i.e., to crystals with essentially ionic bonds between the atoms; but the oxides include minerals with framework (perovskite), chain (rutile, stishovite), and layer (molybdite, plumboxite) structures [4]. Silicates from the chemical viewpoint resemble sulfates, phosphates, etc., and are salts of oxyacids, but the

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