Bulk Modulus and Equation of State under the Effect of High Temperature and High Pressure for MgO

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A new method for the determination of the equation of state is investigated and applied for MgO crystals. The method is developed by using the Hildebrand approximation and an analytical potential form for the overlap repulsive energy derived by Harrison from quantum mechanical considerations. The bulk modulus is also evaluated for MgO in the temperature range 300 – 200 K and down to a compression of $V/V_0 = 0.6$ using an expression based on the Chopelas-Boehler approximation. The results obtained agree well with the ab-initio values determined by Isaak et al.

Key words: Bulk Modulus; Equation of State; Harrison's Model.
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