

## Effects of Mg-Fe<sup>2+</sup> substitution in calcite-structure carbonates: Thermoelastic properties

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### ABSTRACT

In situ X-ray diffraction has been carried out on two siderite samples of different Fe contents simultaneously at high pressure and high temperature in a DIA-type, large-volume apparatus. Unit-cell volumes, measured up to 8.9 GPa and 1073 K have been analyzed using a Birch-Murnaghan equation of state. With  $K_0'$  fixed at 4, the derived equation of state parameters are:  $K_0 = 117(1)$  GPa,  $(\partial K/\partial T)_p = -0.031(3)$  GPa/K, and  $\alpha(K^{-1}) = 1.76(35) \times 10^{-5} + 3.46(62) \times 10^{-8} T$  for end-member siderite, and  $K_0 = 112(1)$  GPa,  $(\partial K/\partial T)_p = -0.026(2)$  GPa/K, and  $\alpha(K^{-1}) = 2.09(23) \times 10^{-5} + 2.97(39) \times 10^{-8} T$  for the Mg-Fe<sup>2+</sup> solid solution with 60 mol% FeCO<sub>3</sub>. These results, along with results obtained previously on magnesite using the same experimental technique, indicate that Fe<sup>2+</sup> substitution for Mg in the  $R\bar{3}c$  carbonates results in a linear increase of the room-temperature bulk modulus and its temperature derivative with increasing Fe content. The bulk modulus increases by more than 10% from MgCO<sub>3</sub> to FeCO<sub>3</sub>. This bulk modulus-composition relationship is mainly attributed to differences in the compressibility of the  $a$  axis with increasing Fe content, even though the  $c$  axis is more than twice as compressible as the  $a$  axis for a given composition. The bulk modulus-volume relationship in the Mg-Fe<sup>2+</sup> carbonates studied is consistent with trends reported in other ferromagnesian minerals, such as oxides, olivines, pyroxenes, silicate spinels, and garnets, in the sense that it deviates from the empirical prediction that the product of  $K_0$  and  $V_0$  is constant. In addition, these observations are consistent with previous suggestions that substitution of alkaline earth elements by the 3- $d$  transition metals may yield a different bulk modulus-volume relationship.