

Elastic properties of alkaline earth oxides

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The elastic properties and their pressure dependence of four B1-type alkaline earth oxides, MgO, CaO, SrO and BaO, are calculated using ab initio FP-LMTO GGA method to elucidate their systematics. It is found from the Cauchy deviation that the interatomic interaction in SrO is nearest to the two-body force and the many-body contribution is largest in MgO. The elastic anisotropy in SrO and BaO are almost same and only MgO has large positive anisotropy under low pressure. The normalized elastic constants c_{ij}' are introduced for more detail analysis. It is found that only c_{44}' and its pressure dependence vary systematically in the four oxides. The elastic properties of alkaline earth oxides are characterized by c_{44} . c_{44} also affects the high-pressure phase relation of these oxides.