THE MURNAGHAN PARAMETERS

In the usual application of linear elasticity theory, the bulk modulus of a crystal is defined as [7]

$$B_{1} = -V \cdot \frac{dp}{dV} = f_{1}(1/s_{\mu\nu}) \quad (4)$$

$$\sigma_{ij}(S_{ijkl}, \tilde{R}) = \bar{\sigma}$$

where $s_{\mu\nu}$ are the single-crystal second-order elastic compliances in the usual matrix notation, σ_{ij} are the stress tensors, \tilde{R} is the rotation matrix, and f_1 is a functional constant dependent upon the crystal symmetry. Note that B_1 , a scalar, is some linear combination of the elements of the second-order elasticity tensor. The Murnaghan parameters are thus given by [see, for example, Ref. 5]

$$B_{0} = \{ B_{1}^{T} \}_{p=0}$$
 (5)

and

$$B_{0}' = \{ (B_{1}^{T})' \}_{p=0}$$
(6)

where the prime refers to isothermal pressure derivative and the superscript T denotes the isothermal value.

It has been shown experimentally [8] that the bulk modulus of polycrystalline aggregates cannot be given by Eq. (4). In light of the Voigt-Reuss-Hill (VRH) approximation [6],