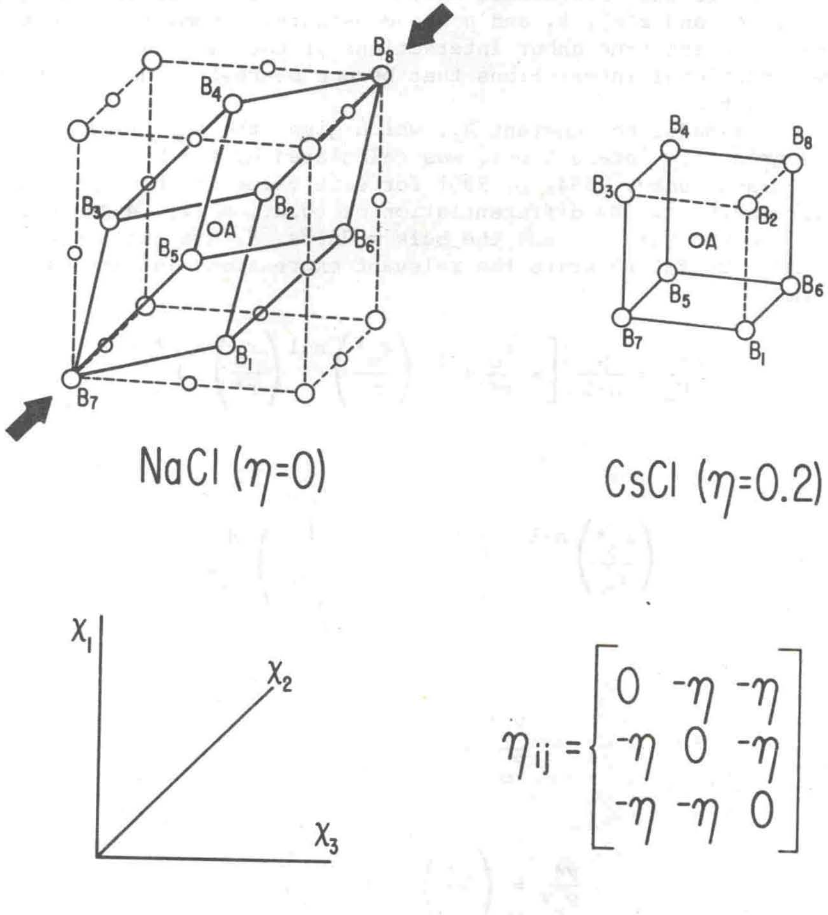
the energy of the lattice as it is continuously transformed from the NaCl to the CsCl structure at a number of pressures, and the results demonstrate the connection between a relatively weak value of C_{44} and the thermodynamic stability of the CsCl lattice. *Hyde* and *O'Keeffe* [1973] used a similar model to study some aspects of this transition, but they did not discuss C_{44}, and limited their calculation to zero pressure.



$$\eta_{ij} = \begin{bmatrix} 0 & -\eta & -\eta \\ -\eta & 0 & -\eta \\ -\eta & -\eta & 0 \end{bmatrix}$$

Fig. 1. Transformation from the NaCl to the CsCl lattice by a shear deformation.

In our model calculation, we ignored thermal effects and assumed that the energy of the lattice is given by the expression

$$F = \frac{z^2 e^2 A_r}{r} + \sum_{i=1}^{8} \frac{b}{r_i^n} \tag{1}$$

where r_i is the interatomic distance, r is the nearest neighbor distance, and z^2e^2, b, and n are constants. Summation is over the six nearest-neighbor interactions of the NaCl lattice and the two additional interactions that become nearest neighbors in the CsCl lattice.

The Madelung constant A_r, which gives the sum of all the electrostatic interactions, was calculated by the Ewald method [*Born* and *Huang*, 1954, p. 385] for each value of the reaction coordinate, η. By differentiation of equation (1), expressions for the pressure, P, and the bulk modulus, K, are obtained. It is most useful to write the relevant expressions in dimensionless form

$$\frac{F^*}{K_o V_o} = \frac{9}{n-1} \left[- \frac{r_o}{r^*} + \frac{1}{N} \left(\frac{r_o^*}{r_o}\right)^{n-1} \left(\frac{r_o}{r^*}\right)^n \right] \frac{A_r^*}{A_r} \tag{2}$$

$$\left(\frac{r_o^*}{r_o}\right)^{n-1} = \left(\frac{6 + 2\left(\frac{r^*}{r_2^*}\right)^n}{6 + 2\left(\frac{r}{r_2}\right)^n} \right) \frac{A_r}{A_r^*} \tag{3}$$

$$\frac{V_o^*}{V_o} = \left(\frac{r_o^*}{r_o}\right)^3 \quad \frac{\beta^*}{\beta} \tag{4}$$

$$\frac{V^*}{V_o^*} = \left(\frac{r^*}{r_o}\right)^3 \left(\frac{r_o}{r_o^*}\right)^3 \tag{5}$$

$$\frac{K}{K_o} = \frac{1}{n-1} \left(\frac{V_o}{V}\right) \left[- 4 \left(\frac{r_o}{r}\right) + (n+3) \left(\frac{r_o}{r}\right)^n \right] \tag{6}$$