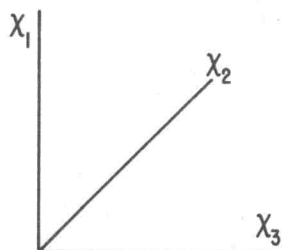
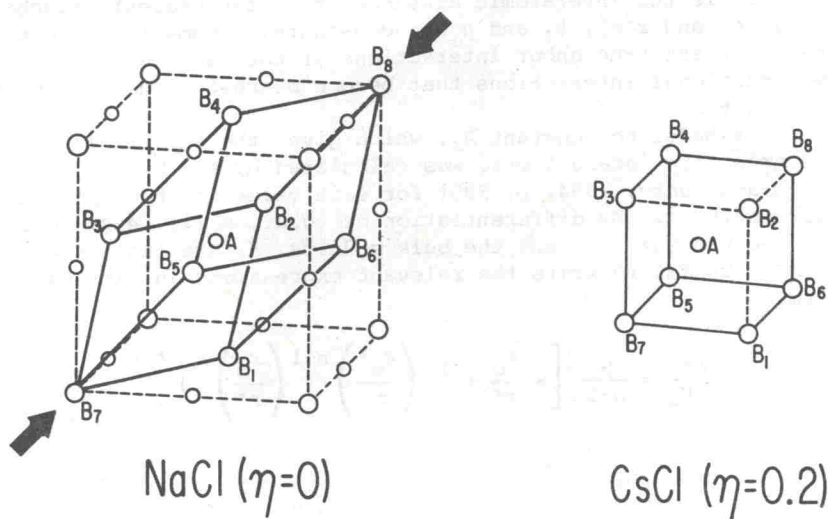


the energy of the lattice as it is continuously transformed from the NaCl to the CsCl structure at a number of pressures, and the results demonstrate the connection between a relatively weak value of C_{44} and the thermodynamic stability of the CsCl lattice. Hyde and O'Keefe [1973] used a similar model 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

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

where r_i is the interatomic distance, r is the nearest neighbor distance, and $z^2 e^2$, 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

$$\frac{F^*}{K_0 V_0} = \frac{9}{n-1} \left[-\frac{r_0}{r^*} + \frac{1}{N} \left(\frac{r_0^*}{r_0} \right)^{n-1} \left(\frac{r_0}{r^*} \right)^n \right] \frac{A_r^*}{A_r} \quad (2)$$

$$\left(\frac{r_0^*}{r_0} \right)^{n-1} = \left(\frac{6 + 2 \left(\frac{r^*}{r_2^*} \right)^n}{6 + 2 \left(\frac{r}{r_2} \right)^n} \right) \frac{A_r}{A_r^*} \quad (3)$$

$$\frac{V_0^*}{V_0} = \left(\frac{r_0^*}{r_0} \right)^3 \frac{\beta^*}{\beta} \quad (4)$$

$$\frac{V^*}{V_0^*} = \left(\frac{r^*}{r_0} \right)^3 \left(\frac{r_0}{r_0^*} \right)^3 \quad (5)$$

$$\frac{K}{K_0} = \frac{1}{n-1} \left(\frac{V_0}{V} \right) \left[-4 \left(\frac{r_0}{r} \right) + (n+3) \left(\frac{r_0}{r} \right)^n \right] \quad (6)$$