

for C_H strain

$$\underline{a}_1 = a \xi^{1/3} (1, 0, 0)$$

$$\underline{a}_2 = a \xi^{1/3} (-1/2, \sqrt{3}/2, 0)$$

$$\underline{c} = c \xi^{1/3} (0, 0, \xi^{-1})$$

$$\text{and } C_H = \left(\frac{d^2 W}{d\xi^2} \right)_{\xi=1} (9/2)$$

A further condition is obtained by considering the first derivatives of the energy with respect to the strains. The conditions for equilibrium with no applied stress are

$$\left(\frac{dW}{d\eta} \right)_{\eta=1} = 0 \quad \text{and} \quad \left(\frac{dW}{d\xi} \right)_{\xi=1} = 0$$

In the case of the C_{66} strain all three contributions have first derivatives which are independently zero; in the case of the C_H strain the Coulomb and the full zone Fermi first derivatives yield negative contributions and must be matched by a positive contribution from the overlap-hole term to comply with the equilibrium condition, which thus becomes an independent and useful condition.

A C_{44} type strain lowers the symmetry of the crystal such that the calculations become quite involved. No attempt was made to account for the C_{44} shear constant.