

APPENDIX

CALCULATION OF FULL ZONE TERM

Following Reitz and Smith⁽²⁾ the energy of the full zone may be calculated by considering the zone to be made up of right tetrahedrons. The contribution to the Fermi energy of each tetrahedron is

$$(W_F^I) = (\alpha_0/4\pi^3)(\hbar^2/2m)(pqr/10) [p^2+q^2/2 + r^2/6] \quad (1)$$

where α_0 is the inverse effective mass of the full zone and p, q, and r are the lengths of the mutually orthogonal edges of the tetrahedron. The lengths p, q, and r may be expressed in terms of the lattice parameter "a", the (c/a) ratio and the pertinent strain parameter, x, such that

$$p = \frac{2\pi}{a} P \left(\frac{c}{a}, x \right)$$

$$q = \frac{2\pi}{a} Q \left(\frac{c}{a}, x \right)$$

$$r = \frac{2\pi}{a} R \left(\frac{c}{a}, x \right)$$

And equation (1) reduces to

$$(W_F^I) = (\alpha_0 \hbar^2 / 10ma^3) [P^2QR + PQ^2R/2 + PQR^2/6] \quad (2)$$