A generalization of Weaire's Hamiltonian shows unrealistic ω-peaks in the density of states even if one takes into account all interactions between nearest neighbour bonds. Treating the bond interaction as a stochastic variable we calculated the CPA-density of states. As expected the ω-peaks are broadened according to the distribution function, while the band gap increases with increasing homogeneity of the solid.

1. INTRODUCTION

In order to investigate the electronic density of states for tetrahedrally coordinated solids like silicon and germanium the tight-binding Weaire-Hamiltonian was extensively studied (see e.g. [1] to [3]). It takes into account the most important nearest neighbour interactions leading to a gap in the density of states between the fully occupied bonding and the unoccupied anti-bonding bands which is responsible for the semiconducting behaviour of the model. This result is independent of the detailed positions of the atoms and the density of states is determined only by the topology of the network.

2. GENERALIZED WEAIRE HAMILTONIAN

We define the Hamiltonian in a 4N-dimensional sp³-orbital representation by means of two interaction operators

\[ S|iR> = \sum_{j \neq i} |jR> \] (interaction at an atom)

\[ T|iR> = |iR> \] (interaction at a bond)

where |iR> is an sp³-orbital centered at atom \( R \) (i = 1, ..., 4) and |iR> is the orbital covalently bound to the orbital |iR>. Taking into account all interactions between nearest neighbour bonds and denoting the interaction integrals according to fig. 1
the Hamiltonian will be
\[ H = V_1 S + V_2 T + V_3 (ST + TS) + V_4 TST \]  
(1)

If the bond lengths and bond angles are the same throughout the network, homologous interaction integrals between nearest neighbour bonds will equally be the same and (1) will be a realistic description of the network provided higher order interactions (e.g. \( V_5 \)) which depend on the dihedral angle between adjacent tetrahedra are unimportant.

Rewriting the Hamiltonian (1) as
\[ H = 4(V_1 - V_4) P + H_2 \]

(where \( P = \frac{1}{2} (S + 1) \) is the \( s \)-projector [3]) one may easily solve the eigenvalue problem of \( H_2 \) in terms of the eigenvalues of the connectivity operator \( T_S = PTP \):
\[ H_2 \phi_{\eta}^\pm = E_{\eta}^\pm \phi_{\eta}^\pm; \quad E_{\eta}^\pm = \pm (V_2 + 2V_3 + 4V_4 \eta) - V_1 + 4V_3 \eta + 3V_4 \]
\[ H_2 \chi_{\eta}^\pm = E_{\eta}^\pm \chi_{\eta}^\pm; \quad E_{\eta}^\pm = \pm (V_2 - 2V_3) - V_1 - V_4 \]

where \( \phi_{\eta}^\pm = P^\pm \phi_{\eta} / \sqrt{(\phi_{\eta}, P^\pm \phi_{\eta})} \), \( P^\pm = \frac{1}{2} (1 \pm T) \) are the bonding and anti-bonding projectors, \( \phi_{\eta} \) are common eigenstates of \( P \) and \( T_S \) (\( P \phi_{\eta} = \phi_{\eta}, T_S \phi_{\eta} = \eta \phi_{\eta} \)), and \( \chi_{\eta}^\pm \) are arbitrary bonding and anti-bonding states completing the \( \phi_{\eta}^\pm \) - set. Since the \( \chi_{\eta}^\pm \) are pure p-states they are eigenstates of \( H \) with \( N \)-fold degenerated eigenvalues at \( \pm (V_2 - 2V_3) - V_1 - V_4 \) yielding the unpleasant \( \delta \)-functions in the density of states.

The integrated density of states may be calculated following John [3] to give (\( E \) with a small positive imaginary part)