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COMMENT

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G A Ringwood

International Centre for Theoretical Solid State Physics, Universitaire Instelling Antwerpen, Universiteitsplein 1, Wilrijk, Belgium

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Abstract. It is deduced, from the analysis of three previous papers on the Weaire model, that topological disorder can only increase the band gap.

It would be natural to guess that the electronic band structure of a crystalline semiconductor would be somehow blurred by any disorder, and that with sufficient disorder the band structure and hence the semiconducting properties of the crystal would be lost. It is shown below that for topological disorder of any degree the band structure of the Weaire model is preserved.

In three previous papers (Lukes and Nix 1973a, b, Carroll *et al* 1974a) a formalism was developed for studying the tight binding Hamiltonian of Weaire (1971) in terms of the number of returning walks. By studying various examples it was concluded that for W-coordinated structures, with all bonds saturated, the asymptotic form of the number $N(t)$ of returning walks of t steps is, in general,

$$N(t) \sim AW^t t^{-3/2} + B(-g)^t f(t)$$

where A, B and g are positive constants, $0 < g \leqslant W$ and

$$t^{-1/2} \geqslant f(t) \geqslant t^{-3/2} \qquad \text{as } t \to \infty.$$

The positions of the inner band edges are determined by $gc = -1$ where

$$c = V_1 V_2 / \{[E-(W-1)V_1](E+V_1) - V_2^2\}, \qquad |V_1/V_2| < 2/W.$$

A graph of c is presented in figure 1 of Carroll *et al* (1974a). The shape of the inner band edges is determined by the form of $f(t)$.

For tetrahedrally bonded solids $0 < g \leqslant 4$, and in particular for a diamond structure $g = 4, f(t) = t^{-3/2}$. With the aid of figure 1 it can be deduced that the diamond lattice has the maximum possible bandwidth and that topological disorder can only increase and not reduce the band gap. Thus in the context of this tight binding model, pure topological disorder (that is, no variation in V_1 and V_2; this corresponds to fixed bond length and angle) to whatever extent cannot destroy the semiconducting property. The effect of variations in V_1 and V_2 on the positions of the band edges is examined by Carroll *et al* (1974b).

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