Electronic Density of States of Amorphous Si and Ge

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The density of states of the valence and conduction bands of Si and Ge are discussed using a simple tight-binding Hamiltonian. It is shown that certain features of the density of states for the case of the diamond structure are related to the short-range order and hence should be retained in the amorphous state while others depend on long-range order and are expected to disappear.

Much recent experimental effort has been devoted to the determination of the electronic density of states of amorphous semiconductors, particularly Ge and Si, and the results so far obtained have excited a good deal of theoretical speculation on the subject. An accurate comprehensive theory for the electronic properties of these solids is still lacking and is likely to remain so for some time. However, it has recently been shown that the problem is not wholly intractable if a simple Hamiltonian of the tight-binding type is used—in particular, it can be shown that for such a Hamiltonian there is a gap in the electronic density of states for any structure with tetrahedral coordination of nearest neighbors. This dispels some, if not all, of the mystery surrounding the observation of such a gap in the amorphous state. In this Letter the same Hamiltonian is used to give a discussion of the shape of the density of states for crystalline and amorphous semiconductors which hinges on a question that has long been of interest in this area but has hitherto been almost entirely unresolved. Which features of the crystalline density of states are due to the long-range order of the structure and which are due only to the short-range order? Only the latter are expected to be retained in the amorphous structure since this
introduced to describe this in a tight-binding formalism.\textsuperscript{11,13} In particular, our model produces another delta function at the top of the conduction band\textsuperscript{11} which in reality (represented by Herman's calculation with sufficient accuracy for our purposes) corresponds to bands that are spread over a wide range of energy.\textsuperscript{11,13} While some apology for the failure of the model to accurately describe the conduction band in the crystalline state seems in order, it should be stressed that the model does give a good description of the valence band and is the only one for which precise and rigorous statements can be made for topologically disordered (i.e., amorphous) structures at the present time.

We assume that the Hamiltonian (1) applies to amorphous systems where the details of the topology or connectivity of the amorphous structure enter through the summation in (1). We thereby neglect the random variation of $V_1$ and $V_2$ due to distortions of bond lengths and angles from ideal values of perfect tetrahedral coordination. While current structural models$^{17}$ support such a viewpoint as a first approximation, the effect of the superposition of this quantitative disorder on the topological disorder which we have studied is certainly worthy of further attention. The delta function in the density of states in Fig. 1 remains even if the structure is disordered—indeed it is quite independent of the details of the structure provided that it is everywhere tetrahedrally coordinated.$^{11}$ The delta function and hence the broadened peak which is found in more realistic calculations are consequences of the short-range order (by which we mean merely the tetrahedral coordination of the nearest neighbors) and not the long-range order; it is not a "Brillouin-zone effect" related to the translational symmetry of the crystal. The delta function contains 2 states per atom for all tetrahedrally coordinated structures and the existence of even rings is not necessary\textsuperscript{11} although these do provide a useful representation for the wave function in the diamond lattice.

The other peaks at the bottom of the valence and conduction bands are indeed Brillouin-zone effects, as may be neatly demonstrated by an exact calculation\textsuperscript{10} of the density of states for the Bethe lattice, also shown in Fig. 1.

The Bethe lattice$^{10-21}$ is a mathematical network containing no closed loops and having a constant coordination number which in this case is 4. It has the advantage of being mathematically tractable, and may be regarded either as a purely abstract lattice having no physical counterpart,\textsuperscript{22} or
as a convenient first approximation in treating real amorphous structures. While the delta function in the density of states for the diamond structure remains for the Bethe lattice, the rest of the density of states is rather featureless as shown by the dashed line in Fig. 1. The two pronounced peaks in the lower half of the valence band for the diamond structure are not found here, which demonstrates that they do not result from the tetrahedral coordination and we may attribute them to the long-range order of the crystal structure. In other words, the broad peak at the top of the valence band is due to short-range order and should be retained in the amorphous state while those at the bottom of valence and conduction bands are related to the long-range order and are not expected in the amorphous state.

Figure 2 presents a sketch of the density of states expected for amorphous Si and Ge on the basis of these considerations. We have also sketched the form of the density of states as suggested by two alternative theoretical models. Brust has proposed that the crystalline density of states, calculated for a dilated crystal and broadened somewhat, is appropriate for an amorphous semiconductor. Our model shows that this is a highly questionable procedure, for although it may be reasonable for the lower part of the valence band in Fig. 1, it is surely incorrect for those states at the top of the valence band that result from short-range order.

Penn has set up a simple isotropic model for the band structure of an amorphous semiconductor, in which the density of states diverges logarithmically on either side of the gap and is free-electron–like elsewhere. Phillips has recently advocated such a model. Of course the logarithmic divergences are assumed to be broadened into two peaks.

The three models represented in Fig. 2 are derived from rather different points of view. The one presented here may be preferable on the grounds that it is based on the study of a Hamiltonian approximating the true Hamiltonian is a well-defined way, rather than on an arbitrary Ansatz. That is not to say, however, that either of the other two approaches might not give a better description of the density of states. All three models would appear to be qualitatively in accord with the density-of-states picture suggested by Donovan and co-workers on the basis of photoemission and optical-absorption measurements, although the fact that no evidence was found for any structure in the conduction band might be regarded as somewhat at variance with the Brust and Penn-Phillips models. All three models entail a broad peak at the top of the valence band, in keeping with the conclusions of Donovan and co-workers. Clearly experimental information concerning the density of states in the lower half of the valence band would be most useful at this point. Unfortunately all the photoemission studies done so far on amorphous semiconductors have not used photons with sufficiently high energies to probe the lower half of the valence band, because of a lack of suitable windows. Soft-x-ray emission spectroscopy, which does not appear to have been used yet to investigate amorphous Si and Ge, should provide a clear and direct indication of the shape of the density of states over the entire valence band, since it is remarkably successful in doing so for crystalline Si. Such a measurement is therefore proposed as a critical test of the model used here. It should not be difficult to discriminate between the three models illustrated by Fig. 2, since their implications for the shape of the valence band are quite distinct.

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Nonexistence of Magnetic Ordering in the One- and Two-Dimensional Hubbard Model

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It is shown that for nonzero temperature, Hubbard's narrow-energy-band model is neither ferromagnetic nor antiferromagnetic in one and two dimensions.

The Hubbard model for the description of electron correlation in a narrow energy band has been of great theoretical interest for the last few years. The model retains only that part of the electron-electron interactions which arises as a result of the repulsion between two electrons of opposite spins located at the same site. In spite of this simplifying assumption, the model remains essentially a many-body problem and an exact solution cannot be found in the general three-dimensional situations. The one-dimensional problem with nearest-neighbor electron transfer has been solved exactly by Lieb and Wu, who obtained the ground-state energy, the wave function, and the chemical potential for the system. In three dimensions Nagaoka considered the case of nearest-neighbor hopping and has discussed the ferromagnetism of various lattices for a nearly half-filled band. Apart from these, not many exact results are known for the model.

In this work we demonstrate explicitly the impossibility of the existence of spontaneous ferromagnetic or antiferromagnetic ordering for this model in one and in two dimensions at an arbitrary nonzero