search & discovery

Model for amorphous semiconductors predicts energy band gaps

How do amorphous semiconductors get their energy band gaps? Experimental results[1,2] over the past few years have shown that amorphous silicon and germanium films have gaps between valence and conduction bands that are similar to the gaps that exist when these substances are crystalline. Efforts to justify these gaps theoretically bog down because of the lack of Bragg planes in amorphous substances; energy band gaps in crystals arise because of scattering by the planes, and most solid-state theorists have assumed that some kind of periodicity is needed to explain gaps.

Now Denis Weaire, a theorist at Yale, has come up with a simplified mathematical model that predicts the gaps.[3] Weaire gets exact bounds on the density of states for his model Hamiltonian, which represents a nonperiodic tetrahedral network. Here every silicon or germanium atom is in perfect tetrahedral coordination with its nearest neighbors, but longer-range neighbors are distributed randomly; previous calculations of the electronic structure of amorphous systems had added disorder to a basically periodic structure. Real amorphous films of germanium and silicon are certainly highly disordered, and may very well exist as random tetrahedral arrays after annealing.[4]

Weaire's Hamiltonian

$$\mathcal{H} = \sum_{i,j} V_1 |\psi_i\rangle\langle\psi_j| + \sum_{k,l} V_2 |\psi_k\rangle\langle\psi_l|$$

considers only interactions between mutually orthogonal hybrid sp^3-type orbitals, the usual tetrahedral orbitals described for carbon compounds. Here i and j are two of the four orbitals on the same atom, and k and l are on nearest neighbors. Note that in this simplified expression all bond angles are equal (V_1 is constant) and all bond lengths the same (V_2 is constant); the model does, however, satisfy the covalency needs of the atoms, despite the simplifications.

To look for energy gaps, Weaire considers a particular value of the energy E. According to Schrödinger's equation, $(\mathcal{H}-E)\ \psi = 0$ for an eigenstate of the Hamiltonian, so that there is a zero density of states at E if Schrödinger's equation has no solution at E, or if we are not able to normalize the wave function.

Weaire shows rigorously that, for this Hamiltonian, there are always two allowed bands separated by a gap. In subsequent work he has shown that there are always four allowed states per atom on either side of the forbidden region.[5] We have, in other words, a band gap between occupied and unoccupied states.

Other theorists have treated electronic properties of disordered systems,

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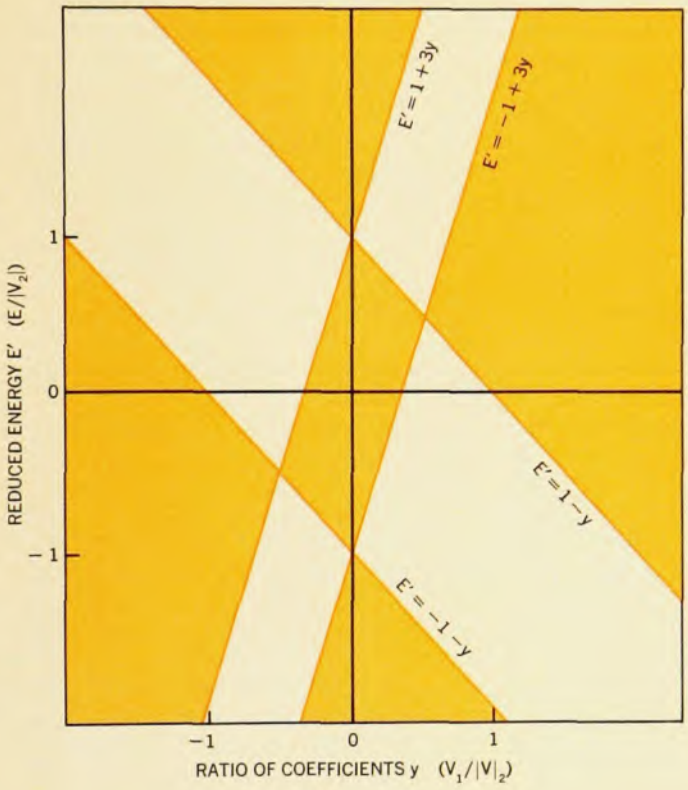

Bounds on the density of states. Here the shaded regions are forbidden (density of states is zero), and the unshaded regions are allowed.

Cosmic-ray muon flux and the W particle

Four years ago Jack Keuffel and his collaborators at the University of Utah found an anomalous muon flux in cosmic rays. Their recent results are consistent with the observation of a W particle, or intermediate vector boson, whose mass is estimated at 20 to 40 GeV. The W particle is believed to be the carrier of the weak force, with a role comparable to that of the pion in nuclear forces. The Utah analysis depends on a model of the W put forth by James D. Bjorken (SLAC), Sandip Pakvasa, San-Fu Tuan and Walter Simmons (University of Hawaii). Results were reported late in August at the International Conference on Cosmic Rays in Hobart, Tasmania and the APS Division of Particles and Fields meeting in Rochester.

Keuffel told us that his group (Haven E. Bergeson, Gerald Bolingbroke, Gary Carlson, Donald Groom, James Morrison and John L. Osborne) is very excited about the result. However he cautioned that many of those attending the two conferences, although interested in the result, have reserved judgment until

ticular regularity that had been expected for the simple induced tensor term, Wilkinson said. "But we no longer expect the proportionality in that simple form; so it could well be that there's a genuine weak-interaction effect that is momentum-transfer independent, or largely so."

In comparing say B^{12} and N^{12}, one must include the effect of the Coulomb force in repelling the positron and pulling back the electron. Wilkinson says that these Coulomb effects can be computed with a reliability of 0.1%, a very tiny error compared to the 10–20% effect observed.

Then there are the possible contributions of higher-order terms. Wilkinson says one would expect there to be asymmetries in mirror transitions caused by ordinary first-class second-forbidden transitions, but you would expect these would amount to only one or two percent. In the mass-12 case, which has been calculated, the effect has a magnitude of 2%, and the wrong sign.

One suggestion to explain the asymmetry regularities, that the asymmetry is always fairly large and always the same sign, is that it is caused by binding-energy differences. For the mass-12 system such calculations had been done, and the effect found was not large enough. Over the past several months Wilkinson has been studying the binding-energy effects. For masses 8, 9, 12 and 13, all in the 1p shell, rather good wave functions are available and so are the data. The calculated binding-energy effect for these systems averages out to about 4%, whereas the experimental average is about 14%.

For masses 17, 20, 24, 25 and 28, all in the sd shell, good wave functions are not available, Wilkinson said. Using a Monte Carlo approach to calculate the binding-energy effect, he concludes that it could not account, again by a factor of 3–4, for the experimental value for the asymmetry for the sd-shell cases either.

The asymmetry may be caused by some systematic wave-function change as you go across each multiplet, Wilkinson says; for example, the deformation might change in a systematic way as you go from neutron-rich to proton-rich bodies, although he doubts that. Calculations are needed in which charge-dependent effects are included in the calculation right from the beginning, rather than put in at the end just as a perturbation.

In summary, Wilkinson said, "One can't say that the induced-tensor term is completely exploded. One can say that if it is producing these asymmetries, its effect in complex nuclei is very different from what you'd calculate simply by taking initial and final-state wave functions for the bound nucleons and sandwiching between the two an operator of the old-fashioned induced tensor type, because that ignores the exchange terms. But we are also very sensitive now to the possibility of some other type of second-class current of an essentially many-body nature."

Many things remain to be done experimentally, but they are difficult. Muon absorption processes can be studied in complex nuclei. (Muon absorption is essentially inverse beta decay.)

One can also study the asymmetry between the beta decay of Σ^+ and Σ^- to Λ^0. Present results are not able to exclude a second-class term of the magnitude that appears to be involved in complex nuclei, Wilkinson said.

In the mass-12 system transition to the first excited state, there appears to be an asymmetry of about -0.1, and those measurements need repeating, Wilkinson says. "If new experiments simply conform to the present systematics, then we're not really getting much further forward. If they give results totally inconsistent with the present systematics, the whole thing might be some sort of bizarre jest on Nature's part." —GBL

References

1. D. H. Wilkinson, Phys. Lett. **31B,** 447 (1970); D. H. Wilkinson, D. E. Alburger, Phys. Rev. Lett. **24,** 1134 (1970); D. E. Alburger, D. H. Wilkinson, Phys. Lett. **32B,** 1390 (1970).
2. J. Delorme, M. Rho, Phys. Lett. **34B,** 238 (1971).
3. H. J. Lipkin, Phys. Rev. Lett. **27,** 432 (1971).
4. D. H. Wilkinson, D. E. Alburger, Phys. Rev. Lett. **26,** 1127 (1971).

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such as *compositionally* disordered alloys.[6] The significance of Weaire's contribution is that he comes up with an *exact* result that predicts the band gap in a *topologically* disordered system. "I have essentially shown," he explained to us, "that the broad features of the band structure are not at all affected if we do not have a periodic structure." He compared his approach with that of a chemist, in contrast with a solid-state physicist: "Chemists think that short-range interactions are all that matters, and solid-state theorists like periodicity. In this case, the chemists have been shown to be right."

Weaire's model is, of course, oversimplified—as he himself points out—and neglects the bond-angle and atomic distortion present in real elemental semiconductors. Details of what happens at the band edges, for example, are not described by the model. Weaire notes that, although his results are not compatible with the existence of localized states throughout the gap, these states could be introduced by defects or by slight fluctuations in bond configurations. Morrel Cohen (University of Chicago) and others have discussed the existence and character of such states, but, stresses Weaire, "this is at a much more detailed level than what I have done here."

Experimental studies of amorphous semiconductors do not settle the questions about the density of states at band edges, as was brought out at the conference on amorphous and liquid semiconductors that took place in Ann Arbor, Michigan this August. (Proceedings will be published as a special issue of the *Journal of Non-crystalline Solids.*) Several groups reported optical-absorption data. William Spicer (Stanford), Terence Donovan and Jack Fisher (US Naval Weapons Center, China Lake, Cal.) for example report that, in amorphous germanium, the absorption falls very rapidly at a particular energy. Marie-Luce Theye (Orsay) has also found sharp band edges, but at a significantly different energy from the California group. Other experimentalists have found exponential rather than sharp edges.

A problem in the experimental studies has been controlling the detailed structure of the films; the kind and degree of disorder introduced into the films has been difficult to evaluate. One promising new approach comes from Walter Spear (Dundee University), who has been measuring transient drift mobility and field effects in amorphous films. He is now sorting out the density of states within the band gap into a part that is independent of the details of film preparation (ideal) and a part that is not (and therefore depends on defects and impurities). When this kind of result can be correlated with optical absorption data, then more precise comparisons between experiment and theory will be possible. —MSR

References

1. T. M. Donovan, W. E. Spicer, Phys. Rev. Lett. **21,** 1572 (1968).
2. T. M. Donovan, W. E. Spicer, J. M. Bennett, Phys. Rev. Lett. **22,** 1058 (1969).
3. D. Weaire, Phys. Rev. Lett. **26,** 1541 (1971).
4. S. C. Moss, J. F. Graczyk, Phys. Rev. Lett. **23,** 1167 (1969); D. E. Polk, J. Noncryst. Solids **5,** 365 (1971); N. J. Shevchik, Bull. Am. Phys. Soc. **16,** 347 (1971).
5. D. Weaire, M. F. Thorpe, Phys. Rev. B **4,** 2508 (1971).
6. M. H. Cohen, *physics today*, May 1971, page 26. □