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$$\sigma(\beta/2) = \left\{ (1/N) \sum_i \left[\frac{\ln A - \ln \pi_i}{R_i} - \frac{\beta}{2} \right]^2 \right\}^{1/2} \quad (6)$$

where π_i is the pathway coupling to site i in the protein, which contains N nonhydrogen atoms.
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Compressibility of Solid C_{60}

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Room-temperature powder x-ray diffraction profiles have been obtained at hydrostatic pressures $P = 0$ and 1.2 gigapascals on the solid phase of cubic C_{60} ("fullerite"). Within experimental error, the linear compressibility $d(\ln a)/dP$ is the same as the interlayer compressibility $d(\ln c)/dP$ of hexagonal graphite, consistent with van der Waals intermolecular bonding. The volume compressibility $-d(\ln V)/dP$ is $7.0 \pm 1 \times 10^{-12}$ square centimeter per dyne, 3 and 40 times the values for graphite and diamond, respectively.

THE RECENT DISCOVERY OF AN EFFICIENT synthesis of C_{60} and C_{70} has, among other things, facilitated the study of a new class of molecular crystals ("fullerites") based on these molecules ("fullerenes") (*1*). The first x-ray powder diffraction profile of solid C_{60} was analyzed in terms of a faulted hexagonal close-packed (hcp) lattice (*1*), consistent with close packing of spherical molecules but with weak second-neighbor intermolecular interactions. A more recent single-crystal study shows that the molecules are actually centered on sites of an unfaulted face-centered cubic (fcc) Bravais lattice but with a high degree of rotational disorder (*2*). With either indexing, the center-to-center distance between neighboring molecules is 10.0(2) Å, implying a van der Waals (VDW) separation of 2.9 Å for a calculated C_{60} diameter of 7.1 Å (*3*). Nuclear magnetic resonance (NMR) spectroscopy clearly indicates the existence of dynamical disorder (presumably free rotation) which decreases with decreasing temperature (*4*, *5*). More work is needed to reconcile conclusions pertaining to dynamic effects on the different time scales of x-ray and NMR experiments.

The nature of intermolecular bonding is of considerable interest, both in its own right and as a clue to the potential electronic properties of fullerites and their derivatives. One expects a priori that the bonding would consist primarily of VDW interactions, analogous to interlayer bonding in graphite. Isothermal compressibility is a sensitive probe of interatomic-intermolecular bonding in all forms of condensed matter and also provides a check on the potentials used in molecular dynamics simulations. We have performed such an experiment on pure solid C_{60}, using standard diamond anvil techniques and powder x-ray diffraction. We find that, within experimental error, the linear compressibility $d(\ln a)/dP$ of cubic C_{60} is the same as the c-axis or interlayer compressibility $d(\ln c)/dP$ of graphite. This indicates that the functional relations between energy and close-packed layer separation are similar in the two solids.

We used standard techniques to prepare our powder sample: soot production by "burning" graphite rods in 300-torr He, Soxhlet extraction in boiling toluene, and liquid chromatography in hexanes on neutral alumina (*6*). High-performance liquid chromatography (HPLC) with a Pirkle column (*7*) showed >99.5% pure C_{60}. The resulting powder was dried in flowing N_2 at 400°C to drive off all traces of solvents. Preliminary powder diffraction profiles were consistent with an fcc cell, $a = 14.1$ Å, with no detectable peaks from other phases. A small amount of powder was packed into a hole 1 mm in diameter in a stainless steel gasket 0.6 mm thick, located between the anvils of a standard Merrill-Bassett diamond anvil cell (DAC). A hydrostatic environment was assured by filling the remaining volume with a 50:50 mixture of ethanol: methanol. Attempts to incorporate a small amount of powdered solid with known compressibility along with the fullerite were unsuccessful; after several tries, we were unable to produce a usable combination of relative scattering intensities, clearly defined peaks, and measurable pressure shifts using any of the usual standards. Thus we resorted to a secondary pressure scale based on the torque of the three screws that compress the liquid and deform the gasket (as established in previous experiments). After measuring the fullerite at "high" pressure, we reloaded the cell with graphite powder, using an identical gasket, and measured the position of the graphite (002) reflection at the same torque settings used for the fullerite measurements. This procedure established that the torque-pressure relation conformed to the secondary standard to within 10%.

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We measured powder profiles in the DAC using a two-axis diffractometer consisting of a Mo rotating anode operating at 7.5 kW, a focusing graphite (004) monochromator, a Soller slit after the sample, and a NaI scintillation detector. The longitudinal resolution ΔQ was about 0.05 Å^{-1} full width at half maximum. The positions of the three strongest peaks of solid C_{60} [the (111), (220), and (311) reflections], recorded at 0 and 1.2 GPa, were fitted to the predicted values for an fcc lattice with *a* as an adjustable parameter. The results are shown in Fig. 1.

Two differences are noticeable between the profiles at 0 and 1.2 GPa. First, at higher pressure all the peaks shift to higher *Q*, indicating a reduction in lattice constant. Furthermore, the relative intensities of (111), (220), and (311) reflections exhibit significant pressure dependence. This can be understood in terms of the unusual structure factor (described below) and a decrease in $\bar{a}$ with fixed C_{60} diameter. A similar change in relative intensity occurs at low temperature and $P = 0$ GPa due to thermal contraction (*8*). Scans at intermediate torque values indicate that both of these changes are monotonic with increasing pressure and that the *P*-induced shift is reversible upon release of the torque.

The profile fits in Fig. 1 show that *a* has decreased by 0.4 Å between 0 and 1.2 GPa. If there is no change in molecular radius, this corresponds to a reduction in intermolecular spacing from 2.9 to 2.5 Å. The *a*-axis compressibility $-d(\ln a)/dP$ is 2.3×10^{-12} cm^2/dyne, essentially the same as the interlayer compressibility $-d(\ln c)/dP$ of graphite within our combined 10% experimental error on *P* and *a*. The system retains the fcc structure up to at least 1.2 GPa, so it is reasonable to assume that all the volume reduction is accommodated by decreasing the VDW separation between molecules rather than by compressing or deforming the spheres. This is also consistent with the fact that a pressure of 1.2 GPa has no measurable effect on the in-plane lattice constant of graphite (*9*).

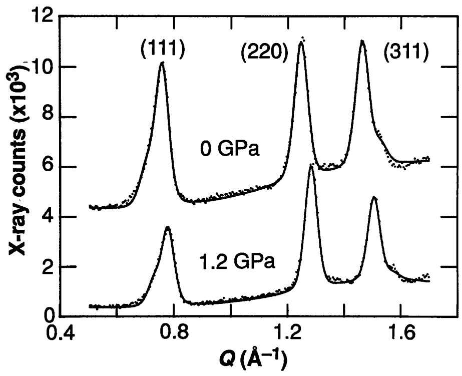

Fig. 1. Powder x-ray profiles of solid C_{60} at atmospheric pressure (top) and 1.2-GPa hydrostatic pressure (bottom). Dots are experimental points (approximately 70 per point), and the solid curves are least-squares fits to an fcc structurewith adjustable lattice constant *a*. The fitted relative intensities have no physical significance in this simple model. The scattered wave vector $Q = 4\pi\sin\theta/\lambda$, where θ is the Bragg angle; for these profiles wavelength $\lambda = 0.71$ Å. Indexing of the strongest peaks is indicated. The high-Q shoulder on the (311) is the weak (222) reflection; the low-Q shoulder on the (111), observed to some extent in all our nominally pure C_{60} samples, is presently unidentified. The variable intensity of this shoulder has little effect on the lattice constant of a particular sample, so we can safely conclude that it has no effect on the compressibility derived from the present data.

At both atmospheric pressure and 1.2 GPa, the (111), (220), and (311) reflections are observed with comparable intensities but there is no detectable (200) intensity (expected near 0.9 Å^{-1}). This is unusual for fcc structures but can be understood in terms of the x-ray form factor. If we assume, as suggested by NMR results, that the C_{60} molecule is freely rotating at room temperature, then its ensemble-averaged charge density is that of a spherical shell of charge. The Fourier transform of a uniform shell of radius R_0 is $j_0(QR_0) = \sin(QR_0)/QR_0$, where j_0 is the zero-order spherical Bessel function. This ad hoc form factor in fact describes the data very well. Figure 2 shows a powder profile recorded over a wider range of scattering angles and with higher resolution than the DAC profiles (*10*) (Fig. 1), along with a fit to a model consisting of shells with 3.5 Å radius centered on fcc sites but neglecting translational thermal disorder. The excellent agreement indicates that the C_{60} molecules exhibit little or no orientational order at 300 K, 1 atm. In principle, the disorder could be either dynamic or static; the molecules could be spinning rapidly, as inferred from NMR measurements (*4, 5*), or the symmetry axes of the icosahedral molecules could exhibit no site-to-site correlation in their directions. Either conjecture is consistent with the fact that a single-crystal refinement at 300 K fails to localize the polar and azimuthal angles of individual C atoms (*2*). The absence of detectable (200) intensity (and, indeed of any (*h*00) peaks with *h* even) is entirely due to the fact that $j_0(QR_0)$ has minima at the corresponding Q values if $R_0 = 3.5$ Å and $a = 14.11$ Å.

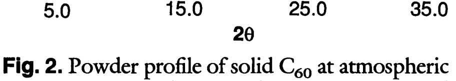

Fig. 2. Powder profile of solid C_{60} at atmospheric pressure, measured on a diffractometer equipped with a position-sensitive detector (*8*) and a 1.5-kW sealed Cu source monochromatized by the (002) reflection of graphite ($\lambda = 1.54$ Å). The powder sample was contained in a Lindemann capillary tube (0.7 mm in diameter). Dots are the measured points (2 hours accumulation), and the solid curve is a least-squares fit to an fcc lattice of uniform spherical shells. The best-fit parameters are $a = 14.11$ Å and shell radius $R_0 = 3.5$ Å. This sample exhibits much less intensity in the low-angle shoulder of the (111) reflection.

Kratschmer *et al.* noted (*1*) that the inferred VDW C diameter in solid C_{60} (2.9 to 3.0 Å) is considerably less than the 3.3 Å value characteristic of planar aromatic molecules and graphite. The observation of different diameters yet similar compressibilities can be rationalized qualitatively as follows. Intermolecular or interlayer separations in C_{60} and graphite, respectively, are determined by the balance between attractive and repulsive energies, whereas the corresponding compressibilities are defined by gradients of these energies. It is easy to show that the number of VDW bonds per unit area parallel to a close-packed layer is only 1/7 as large in C_{60} as in graphite (if neighboring C_{60} molecules orient with adjacent hexagonal faces in opposition). This implies a large difference in the total energies of the two solids but does not directly account for the reduced VDW separation; if the close-packed layers were very stiff, the equilibrium spacing would be independent of bonds per area. However, the nature of the bonds is qualitatively different. The lobes of p_z charge in fullerene are normal to the spherical surface and probably remain nearly so in the solid. This orbital structure permits a closer approach of neighboring C_{60} molecules as compared to the spacing in graphite because the lobes extending into the intermolecular gap in C_{60} are "splayed out" with respect to a normal to the close-packed plane rather than strictly normal to the plane as in graphite. Simple trigonometry shows that this effect alone can account for more than one half the reduction in the VDW separation.

The p_z splaying also adds a new repulsive contribution to the total energy relative to that of planar systems. In graphite, a small reduction in interlayer spacing compresses the π charge; in fullerite there would also be a tendency to increase the splay angle, which requires an energetically unfavorable hybridization between pi and sigma orbitals. The VDW "bonds" in fullerite are thus stiffer and shorter, as well as less dense, than in graphite. We propose that the reduced gap is due to the combination of shorter bonds and reduced areal density, whereas the comparable compressibilities result from cancellation between different bonds per area and bond strengths. A direct test of this proposal can be performed if these experiments are extended to higher pressure; if the C_{60} bonds are indeed stiffer than in graphite, the compressibility should decrease rapidly with increasing P.

Isothermal volume compressibilities $-1/V(dV/dP)$ are 6.9×10^{-12}, 2.7×10^{-12}, and 0.18×10^{-12} cm^2/dyne for solid C_{60}, graphite, and diamond, respectively. Clearly, fullerite is the softest all-C solid currently known. The linear compressibility normal to the close-packed planes is nearly equal for solid C_{60} and graphite (*11*). This suggests that there should be no elastic impediments to the formation of "intercalated" (*12*) fullerites.

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A Neuron-Silicon Junction: A Retzius Cell of the Leech on an Insulated-Gate Field-Effect Transistor

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An identified neuron of the leech, a Retzius cell, has been attached to the open gate of a *p*-channel field-effect transistor. Action potentials, spontaneous or stimulated, modulate directly the source-drain current in silicon. The electronic signals match the shape of the action potential. The average voltage on the gate was up to 25 percent of the intracellular voltage change. Occasionally weak signals that resemble the first derivative of the action potential were observed. The junctions can be described by a model that includes capacitive coupling of the plasma membrane and the gate oxide and that accounts for variable resistance of the seal.

MULTISITE RECORDING OF THE electrical activity of neurons is a prerequisite to the study of signal processing in arborized neurons and in neural nets. Such a method must be noninvasive and should detect changes in intracellular voltage at a high spatial and temporal resolution. Optical recording by voltage-sensitive dyes (*1, 2*) and electrical recording by extracellular metallic electrodes on glass (*3–6*) or Si (*7, 8*) have been used. We report on a direct coupling of neural excitation and electrical current in Si in a transistor-type device. The assembly is a first step toward multiple recording in neurons and neural nets and toward the development of neural biosensors and neuroelectronic circuits.

A neuron is mounted on a thin insulating layer of a gate oxide on *n*-type Si in an electrolyte (Fig. 1). A positive-bias voltage is applied to the bulk Si to provide an accumulation of mobile, positive defect electrons near the surface (strong inversion). The positive voltage change in the neuron during an action potential lifts the surface potential of Si and reduces the density of mobile defect electrons. The neuron-Si interaction causes a modulation of the current along the inversion layer (*p*-channel) driven by a voltage between source and drain. The junction thus behaves like a field-effect transistor (FET).

The neuron-FET junction has certain features: (i) direct coupling of neuron and Si owing to an interaction of cell membrane and gate oxide without interfering metal; and (ii) well-defined structure and function made possible by the controlled attachment of an identified neuron to a microscopic transistor of matched design. These features can be compared to the characteristics of earlier approaches: A large (1 mm by 50 μm) FET with an open gate was used by Bergveld *et al.* to record extracellular voltage in muscle tissue (*9*). An FET with a metallized gate was used by Jobling *et al.* (*10*). An assembly of neuron and metallized Si was described by Regehr *et al.* (*11*).

Retzius cells (diameter about 60 μm) were isolated from segmental ganglia of the leech *Hirudo medicinalis*. The soma of the neuron together with a short neurite was dissociated after enzymatic treatment of opened ganglia (*12, 13*). In freshly dissociated cells the amplitude of the action potentials was 40 to 60 mV. Planar technology was used to fabricate *p*-channel insulated-gate FETs (*14, 15*). Source and drain were made on the (100) surface of *n*-Si by boron diffusion. The length of the channel between source and drain was 6 μm. Its width was 30 μm (Fig. 2). The channel region was insulated by a gate oxide 20 nm thick. A Perspex chamber was fixed on the Si plate (*16*). After the gate had been coated with poly-L-lysine, we filled the chamber with electrolyte (leech Ringer, pH 7.4). A neuron was attached on the tip of a glass pipette and mounted on the gate under visual control (Fig. 2) (*17*).

We performed four types of measurement (*18*) with the junctions (Fig. 3). (i) A single action potential was stimulated by current

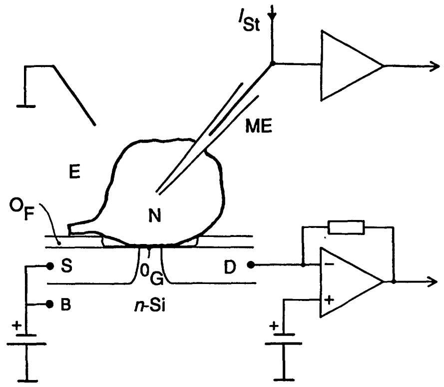

Fig. 1. Neuron-Si junction (unscaled). A neuron (N) is attached to oxidized Si. A thin layer of gate oxide (O_G, marked by the heavy line) covers *n*-type Si between the source (S) and drain (D) of *p*-type Si insulated by a thick field oxide (O_F). The electrolyte (E) is maintained at ground potential (Ag/AgCl electrode). Bulk silicon (B), source, and drain are held at positive bias voltages (*p*-channel FET). The source-drain current is measured by a current-voltage converter. The neuron is impaled by a microelectrode (ME) (Ag/AgCl). Current (I_{St}) is injected to stimulate the cell. The membrane potential is measured by a voltage follower.

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