For the First Time, You Can See Atoms

Roald Hoffmann

We were making a television course, "The World of Chemistry." There was too little money and too little time to do it perfectly. Yet two teams of talented, dedicated people were trying—a group of chemists and teachers, and a television production team. It was, as I learned, an infinitely complicated process, engaging the skills and trades of 30 people, sometimes at loggerheads, as in the production of an opera, banging into shape a piece of video art about chemistry.

Because our budget was so small, we were dependent on "stock footage," a euphemism for free film from industrial or government sources. One video tape that came our way from IBM was about the scanning tunneling microscope, or STM. The microscope is a marvelous technique for studying surfaces, invented by Gerd Binnig and Heinrich Rohrer at IBM's Zurich Research Laboratories. The technique is appealingly simple, and the images it produces so revealing that the invention was immediately recognized as of value, and honored by the 1986 Nobel prize only three years after the work was published.

In the film our television people obtained, IBM, justifiably proud, turned on the hype. Now, for the first time, one could see atoms. Their tape showed a striking, false-color "fly-by" across the surface of a silicon crystal.

To the television production team, daunted by the task of depicting something as intangible as the atom, the IBM footage was a godsend. They made it the centerpiece of a sequence that began with the incredibly beautiful footage of an earthrise on the moon filmed by the Apollo astronauts, evoking the importance of the moon landing—a voyage, a search, a discovery. All the directors' skill, a skill I greatly admired, shaped implicit and overt connections to the STM images. The struggle to form an atomic theory, from Democritus through Dalton, culminated in those appealing pictures of the silicon surface. Now, after such a long time waiting—thousands of years—now, we could see atoms.

I nearly went through the roof (which was high up; we were filming in the New York Hall of Science, an innovative science museum built in a structure remaining from the last New York World's Fair). What treason here to 180 years of theory and experiment that through tedious, indirect evidence built a framework of incontrovertible reality for atoms and molecules! That wondrous scanning tunneling microscope would never have been built, I screamed quietly, were it not for the painfully won, indirect, but certain knowledge that atoms combine into molecules and extended arrays with precise, known geometries.

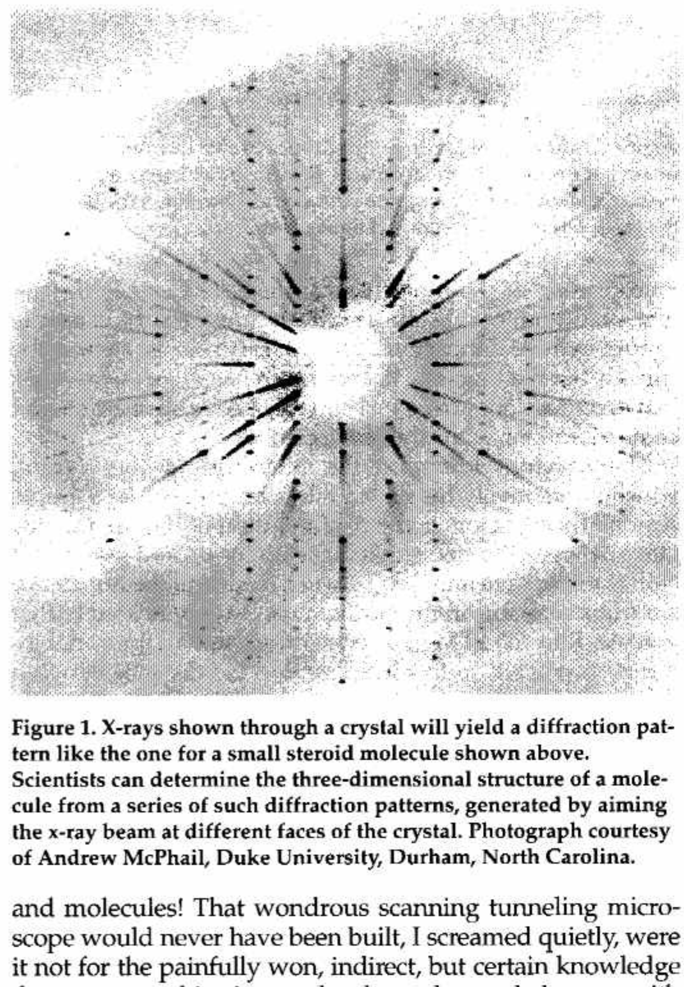

Figure 1. X-rays shown through a crystal will yield a diffraction pattern like the one for a small steroid molecule shown above. Scientists can determine the three-dimensional structure of a molecule from a series of such diffraction patterns, generated by aiming the x-ray beam at different faces of the crystal. Photograph courtesy of Andrew McPhail, Duke University, Durham, North Carolina.

The STM does not really "see." It measures the flow of electrons across the small vacuum gap between a sharp tungsten tip and the surface whose molecular structure is to be determined. The tip, which is much like a phonograph needle, is brought extremely close (within a few Ångströms, or hundred-millionths of a centimeter) to the substance being studied. When a small voltage is applied between the tip and the surface, some electrons jump across the gap using a quantum mechanical mechanism called tunneling. Roughly, the closer the tip to the surface, the greater the current. With tremendously fine control, the tip is moved laterally across the surface, and the current is recorded, stored, computer-enhanced and plotted out, often in a color-coded display that offers a

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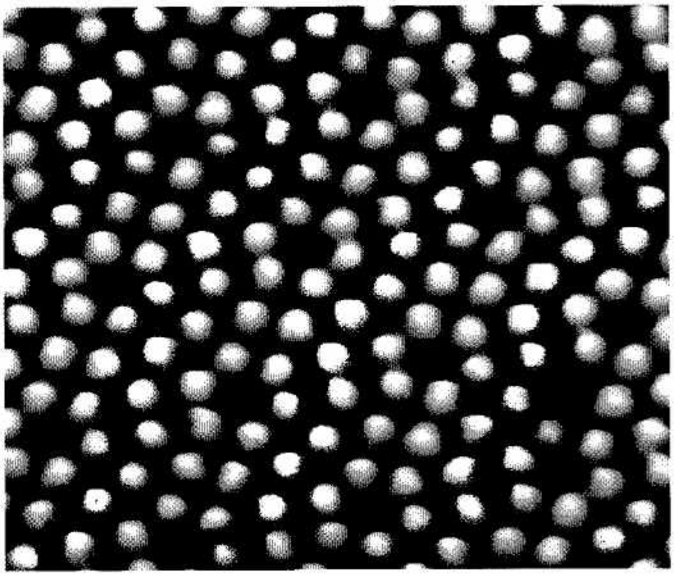

Figure 2. Scanning-tunneling microscopes (STM) can generate images of the surfaces of molecules, like the STM image of a silicon surface shown here. Photograph courtesy of Phaedon Avouris, IBM Research Division, Yorktown Heights, New York.

kind of map of the molecule's surface. The key to this remarkable atomic-scale topographic technique is the exquisite control in three dimensions. The tip has to be just so near the surface, but not touching it, and it then has to move precisely in two dimensions across that surface. Above all, there should be no vibrations while this is happening.

Many factors determine the magnitude of the current, which is eventually translated into a bright spot on a graph. Among those factors is the configuration of the tip, the distance between the atoms that make up the tip and the surface atoms, the voltage imposed between them and the number of electrons available in the surface at an energy related to that voltage. Run the STM in a certain way, and all the variables can be averaged, so to speak, leaving the distance between the tip and the surface (or the height of the atoms above or below the average surface level) as the prime determinant of the current. This is the "topographic" mode, and here one stands the best chance of translating the current observed into an elevation in the surface.

STM studies have made possible remarkable pictures, especially of metal and semiconductor surfaces. For instance, when a certain silicon surface is cleaved out of a crystal, some bonds are broken (the pristine surface is damaged goods). It heals itself by some atoms jumping up above the original surface, many others moving a little or a lot, in a complicated pattern that involves no less than a block of 98 silicon atoms. This wondrously complex "reconstruction" was first shown to us in atomic detail by the STM.

As much as I value the knowledge the STM gives (and I've recently written, together with Boris Schubert and Phaedon Avouris, three papers trying to interpret the beautiful STM pictures of the silicon surface attacked by oxygen), I know it does not "see." When we are lucky, the process produces an image related to the surface topography. Sometimes we are not lucky. We know that graphite layers contain a simple hexagonal honeycomb of carbon atoms. But the STM image of graphite, without fail, shows only triangles, imaging every other atom. There is still a dispute as to what is being seen. But it is not what we know is there.

How, then, do we know? Indirectly, but quite certainly. The structures of most of the metals, alloys and polymers that go into the construction of the STM instrument are known to us through a variety of indirect spectroscopic techniques—instrumental extensions of our senses. Most prominent is the diffraction of x-rays. Here we have about 80 years of experience of working back from a lot of spots (diffraction maxima) on a film to the detailed geometry of a molecule or a solid. Helped by the ubiquitous computer, with a machine costing about 150 kilobucks, a nice small crystal, and a man- or woman-week of work, we can get the structure of a medium-sized molecule. A protein takes longer. What the STM allows is the (indirect) imaging of imperfect, non-repeating structures, of structure in states of matter that are not crystalline. It extends the range of the non-seeing from which an ingenious human being reconstructs an image—and then makes himself believe he really saw it.

Meanwhile, back at the New York Hall of Science: The directors ignored my concern—I was just another scientist adding qualifications to what anyone could see. But there was a slot, a minute long, that I had been given in which to close the program and connect it to the next one, on Mendeleyev's periodic table. For that I wrote the script myself. I quickly substituted the following:

> We've looked in this program at the structure of the atom. We've described the experimental and theoretical steps leading to our modern picture of the atom, this electron cloud around a nucleus. And we saw one technique, scanning tunneling microscopy, for seeing atoms. Only when we understand and see atoms, you might think, only then could we, should we, go on to the next level of complexity, to molecules.
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> Do you think that's true? That development of a field should await complete understanding of its foundations? I hope you don't. We knew the earth was round centuries before Apollo astronauts took a picture of it from the moon. And we were dead sure of the existence of atoms, and knew just how atoms connected up to form molecules, before those beautiful clear STM pictures.
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> Chemistry, like any human activity, proceeds simultaneously on many levels, with partial understanding, always incomplete, sometimes wrong, incredibly, mostly right. A great intellectual achievement of chemistry, of humanity, a chart organizing all the elements, called The Periodic Table, developed 50 years before we knew what the atom is about, is the subject of the next program.

Not only were the directors aghast at what I said, but I also said it well, with feeling. Most of the time I was not good on camera, and there was no money to send me to acting school. So I had their attention, finally. They edited out part of the offensive moon landing–STM sequence. I modified my ending. And we all understood (I think) the point that you do not have to see something to know, as sure as anything, what is in this world.