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Integrated Circuits the Size of Molecules

"In ten years potentially, we will have entire computers not just in your wrist watch, but woven into our clothing. Or a slurry of computers painted on your wall."

Phil Kueckes, Computer Architect, Hewlett-Packard Laboratories, Palo Alto, California, July 1999

August 18, 1999 Palo Alto, California In mid-July 1999, Hewlett-Packard Labs and the University of California at Los Angeles made headlines with a breakthrough that seems like science fiction making integrated circuits for computers no bigger than molecules. Currently, the on-off switches for computing are made by etching pathways with beams of light on silicon wafer chips. But light has a wavelength and cannot make anything smaller than that wavelength.

The researchers say they have now figured out how to use chemistry, not light, to make wires and switches as small as molecules. "This is about as small as we're going to get things," said Phil Kuekes, a computer architect at Hewlett-Packard Laboratories in Palo Alto, California who also earned a physics degree from Yale University in 1969.

Recently I talked with Mr. Kuekes by telephone at his office in Palo Alto and asked him to explain how chemistry can be used to make molecule-size wires and switches.

Interview:

Phil Kuekes, Computer Architect, Hewlett-Packard Laboratories, Palo Alto, California: "The first thing is that the entire chip won't be a molecule. But the switches, the gates, the parts of the chip will be molecules. And we'll put a large number of those together to make the chip.

BUT HOW DO YOU GET DOWN TO MOLECULES?
Molecules are made of atoms. They are a collection of atoms that are stable, you can build and they'll hold together. So, if I were a computer scientist and I wanted to build a really small computer, I would realize that fundamentally I couldn't get any smaller than atoms. So, suppose I were looking around for somebody to work with me in the 21st Century to build things out of atoms to order?

Well, it turns out there's a perfectly good and honorable name for such people for about the past 150 years. We call them chemists. So, chemists are people who really do know how to build something to order on an atomic scale. The problem is that what chemists can build are relatively simple molecules, while biology can create extremely complex things. And we need a designer of a computer to be able to say: 'This is what I want. Create it, no matter how complex.'

So, what our work has done is to produce things much smaller than the wavelength of light or even x-rays which would be required for the lithographic process. We have found a way to use relatively simple molecules and then later on have a computer program add the complexity. So, the manufacturing happens in two steps. You create a simple chemical structure - almost crystalline - and then all the complexity of a modern computer chip gets downloaded in a second step.

What we're doing is using chemically synthesized wires that can be made much smaller than lithographic wires. Long term, these will become the carbon nanotubes we have written about about which are in fact only a few atoms across.

IT ISN'T REALLY WIRE?
Oh, it's wire and it's long and they conduct. They are metallic. The carbon nanotubes are in fact the most conductive substance known on earth. But they are chemically synthesized. So to some extent, what we're talking about are long crystals of metals which are wires. That's what we mean by wires - it's long and narrow and it conducts electricity.

BUT IF WE COULD SEE IT, WOULD THE MOLECULE SIZE WIRES RESEMBLE VERY THIN CRYSTALS?
It's hard to tell the difference. It's relatively stiff, an incredibly stiff thing. It would be more like a bar of metal. It's long and straight and stiff and that's the way that all the wires that are printed on an integrated circuit are. They don't flop around. The silicon is very rigid because it's all bonded to a perfect crystal which is silicon.

But you need switches, and the work we reported in *Science* (www.sciencemag.org/ Pages 391-394, July 16, 1999) allows us to use in principal a single molecule as a switch that can be set open or shut. When it's shut, it conducts electricity. When it's open, it doesn't.

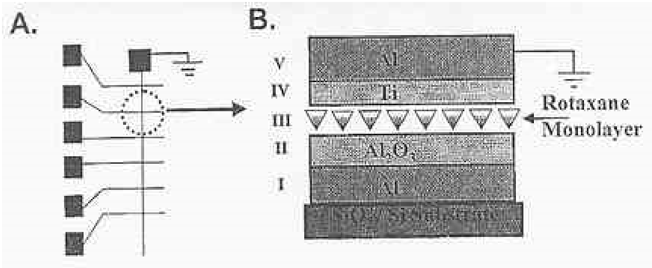
I AM HAVING DIFFICULTY IMAGINING AN OPEN OR SHUT MOLECULE. WHAT IS OPENING OR SHUTTING ON THE MOLECULE FOR A SWITCH?
OK, there are many molecules which have more than one state. The molecules we use actually do change shapes slightly. And so they have two possible states, two different shapes it can be in. And in one of those shapes, it conducts electricity very well through a process which is technically called quantum mechanical tunneling. And in another shape, it doesn't conduct at all. And there is a huge difference in conductivity - potentially as much as 100:1 between the two shapes.

WHAT CHANGES THE SHAPE?
The wonderful thing - and this is what we reported in our paper in Science - if we send pulses down the wires that have a big enough voltage, I can change the shape of the molecule and make it conduct or not conduct. If I use a smaller voltage, then I can actually run it as a computer based on what has been connected or not connected.

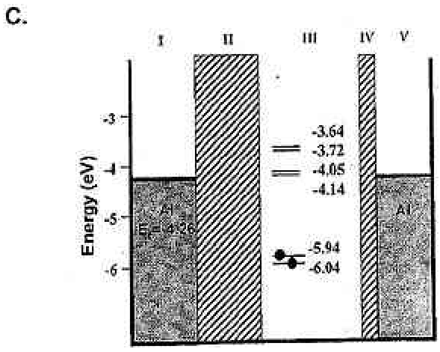
MEANING ZERO OR ONE.
Meaning zero or one, exactly. And that's what we use to build up the complexity of the computer.

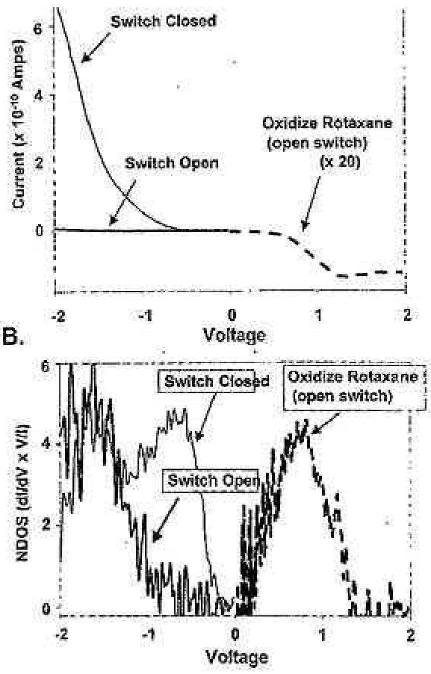
IN TERMS OF THE PARTICULAR SUBSTANCE THAT YOU ARE USING, THAT CHANGES SHAPE THAT ALLOWS ELECTRIC FLOW OR NO ELECTRIC FLOW, WHAT ELEMENT IS IT?
It is not a single element. It is a molecule. It's an organic molecule called Rotoxane. It's synthetic, but it's made of carbon and oxygen and hydrogen and

nitrogen. Rotoxane is organic in the sense that sugar and alcohol or one of those are and it's plastic. So, it's made of the same type of molecules - the same kind of elements - that people mix together when they are making plastics, for example.



Rotoxane molecule, energy and switch mode diagrams © 1999 by Phil Kuekes.





IS PART OF THE BREAKTHROUGH THAT YOU'VE HAD TO COME UP WITH A PARTICULAR ALLOY THAT WOULD HAVE THESE CHARACTERISTICS OF A SHAPE-SHIFTING MOLECULE?

There are several parts to it. So, the first part - I got together with Stan Williams at H. P. Labs, a chemist, and Prof. James Heath at UCLA who is also a chemist. And the first step was to work out a method where chemistry could work with computer architecture. And then given this basic idea that we were going to have chemically constructed wires which were metallic and molecular switches, we started looking around for the wires and switches. We knew that things like the carbon nanotubes would be wires. So, we had to look for a switch. And we got in touch with Prof. Frasier Stoddard now at UCLA who had- for completely other purposes - designed these molecules which changed their shape.

The chemists in the group suspected very strongly - I'm the computer guy - they suspected it would have exactly the electrical properties that we needed to build a computer.

SOMETHING THAT COULD GO ZERO OR ONE, BE TURNED ON BY ELECTRICITY OR BE TURNED OFF BY ELECTRICITY.
That's exactly right. So, the important breakthrough was that we found that we had all the properties we needed in a single molecule. That's important.

BUT DID YOU CONSTRUCT OR DID THE OTHER SCIENTISTS CONSTRUCT THIS MOLECULE SPECIFICALLY FROM SCRATCH TO TRY TO ACCOMPLISH THIS ON/OFF TRANSFORMATION?
No, it was constructed from scratch. It was a synthetic molecule. It was constructed in a test tube. However, it was done just because it was an interesting molecule to construct - essentially as basic research. It is a very interesting molecule.

IT IS IN THE PLASTIC CATEGORY?
Yes.

ANYTHING THAT HAS A STRONG CARBON BASE.
Yes, fundamentally anything that has a lot of carbon in it. The carbon is what makes this stuff work.

WHAT ARE THE IMPLICATIONS OF THIS BREAKTHROUGH FOR COMPUTERS OVER THE NEXT TEN YEARS?
Well, let me first talk about two years and what we think we're going to do. In just two years, we are going to take in an area that is as small as where two of the smallest wires anybody can make for an integrated circuit in the lab - and where two of those wires cross, they form a little tiny square. Inside of that square, we are going to build an integrated circuit that is as complicated as one that I actually used in 1970 to build computers out of. This one two years from now won't be a full computer chip, but it will be able to add one and one and get two, or store 16 bits, not 16 megabits. So, we believe we will have a real building block that is an actual integrated circuit far smaller than any transistor anybody else can build today.

So, what does that mean in ten years? Well, in ten years that means potentially that we will have entire computers - not just in your wrist watch, but woven into your clothing. Or a slurry of computers painted on your wall.

WHAT DO YOU ENVISION RIGHT NOW THAT THESE VERY TINY COMPUTERS COULD BE DOING IN TEN YEARS ON CLOTHES AND WALLS?
It will make it possible to have computing power with you, right? Clearly, smart and creative people will create fashion statements - your clothes will be able to change colors and patterns. So, this is a medium that a lot of creative people are going to be able to step up and start using. Your wall maybe becomes your television screen, or your computer screen.

THE ENTIRE WALL RATHER THAN A MACHINE?
Yeah, an entire wall. Because the machines themselves start to disappear.

BECAUSE YOU CAN ACTUALLY 'PAINT' ON WALLS WITH THE MOLECULE SIZE INTEGRATED CIRCUITS?
That's right, and with a huge number of I-Cs that will be able to talk to each other. It's going to make a huge change when they shrink in size and in price.

Once you start using chemistry to assemble a computer, the price is going to drop dramatically.

WHY IS IT THAT CHEMISTRY HAS THE ABILITY TO GO DOWN EASIER TO THE MOLECULAR LEVEL THAN PHOTON ETCHING?
The fundamental reason is that the wavelength of ordinary light like you and I see is absolutely gigantic compared to an atom. It's tens of thousands of times bigger. So, in fact in an attempt to make smaller and smaller things, current integrated circuits are no longer made with ordinary light. They are made with ultraviolet light. And people are talking about x-rays to make them - incredibly powerful x-ray machines.

THE REASON IS TO GET THAT WAVELENGTH SHORTER AND SHORTER?
Yes, you have to get the wavelengths shorter and shorter and that causes a lot of problems. The present technology fundamentally for making integrated circuits is like taking a stencil and spraying paint through it. The light is used to cut through the stencil. An integrated circuit is very complex. There are many levels of stencil that you have to very precisely and mechanically line up. That's why existing integrated circuit factories, the new ones today, are costing a few billion dollars. This very precise mechanical equipment is very, very expensive.

What chemists know how to do is by getting the temperature and pressure in the mixture of chemicals right, they are able to have the molecules come together in a very precise way and essentially only in that way. There will be some that are wrong. But when they are wrong, you can separate them out.

There's no such thing as a sugar molecule or water molecule or plastic molecule with a scratch or bump or smudge on it. Once you make them, they are all absolutely identical. That's not true of lithographic processes.

WHEN YOU HAVE IDENTICAL MOLECULES SUCH AS THIS SYNTHETIC MOLECULE YOU HAVE MADE OUT OF ORGANIC CARBON WITH SOME OTHER ELEMENTS, IT IS THE SAME FROM MOLECULE TO MOLECULE THAT MAKES THE NANOTUBE WIRES.
Connects the nanotube wires. The molecules connect the wires. So, we make two things in the chemistry lab: we're going to make wires and we're going to make the molecule switches. And then we put them together. Chemically.

CAN YOU GIVE A WORD PICTURE OF EXACTLY WHAT YOU ARE WORKING WITH WHEN YOU GET DOWN TO THE MOLECULAR LEVEL OF THE NANOTUBE WIRES AND THOSE MOLECULE SWITCHES.
Basically what we have is one wire and two other wires cross that wire and in between at the cross points, wherever they cross, there are a bunch of molecules. Maybe not one, maybe two, or three or four - but there will be a small number.

THE PART WHERE THE MOLECULES ARE IS THE SWITCH TO THOSE WIRES?
The switch, and I can connect them or not connect them.

BUT EVERYTHING INCLUDING THE WIRES AND THE SWITCHES ARE ONLY MOLECULES IN DIAMETER?
A molecule or a few atoms in diameter, right. Everything will be. Now, what we built today that's in the news and we've actually got working is - we have two very big wires that are tens of thousands, if not hundreds of thousands, of atoms across. But in between those wires, there is a layer of molecules that is exactly one molecule wide. The distance between those two wires in the experiment we have recently done down at UCLA is exactly one molecule. It's only about 20 atoms long. And it works!

IN TWO YEARS, LET'S SAY, WHEN YOU ARE ACTUALLY IN THE

PROCESS OF CREATING THESE FIRST MOLECULE SIZE INTEGRATED CIRCUITS, WHAT PHYSICALLY WILL IT LOOK LIKE?
It's too small to see, that's the first thing. So to some extent, you can never look at it, except with a very special microscope like a scanning tunneling microscope that can see individual atoms.

HOW DOES THIS GET MANUFACTURED?
Right! So, what we're going to do is again what chemists do: fundamentally shake and bake. They arrange things so they get the temperature right and they mix things together which naturally crystallize. So, we're going to use chemical forces to align all the wires properly and get the molecules in the right place.

But then the problem is: how do we connect wires to it? So, we're working with Prof. Paul McKuen at the Univ. of California, Berkeley, who is one of the world experts at attaching probes to individual carbon nanowires and measuring their conductivity. And he's going to use some of his techniques to actually use an extraordinary high powered microscope and connect to our little chip which is impossible to see with ordinary light.

WHEN YOU START MANUFACTURING THESE NEW MOLECULAR INTEGRATED CIRCUITS, WILL IT ACTUALLY BE A CRYSTAL INSIDE THE COMPUTER?
It's crystal-like. I don't want to push the analogy. Certain parts like the wires are actually somewhat crystalline. It's crystal-like in that it's a very regular structure.

PHYSICALLY TO THE EYE I'M ASSUMING THAT ALL THESE MOLECULES IN WIRES AND SWITCHES HOOKED TOGETHER AND CREATING VERY POWERFUL AND SMALL COMPUTERS THEY HAVE TO HAVE SOME KIND OF PHYSICAL SUBSTANCE.
It's going to look something like a film of plastic. The manufacturing process of this may very well be like making something like photographic film. It's very complex, but essentially it's all chemistry. It's very different chemicals all sandwiched together.

THIS IS WHERE IT COULD BECOME ALMOST LIKE FABRIC THAT COULD BE LAYERED ON WALLS, OR SEWN INTO CLOTHES?
Sewn into clothes or maybe it becomes the thread itself. This is so small that the threads may be computationally capable. What we're really talking about here are smart materials. Right now, we manufacture plastic or metal or steel or aluminum or glass or whatever. But those materials are kind of dumb. What if we could combine manufacturing the substance with our molecular integrated circuits so the materials themselves would get smart?

THE MATERIALS WOULD BE SMART HAVING THE ABILITY TO REACT TO LIGHT, TO HEAT, TO TEMPERATURE, TO TOUCH?
Right, exactly. We are going to be able to program them the people who understand computer programs will be able to program these materials to react appropriately.

DO YOU HAVE AN EXAMPLE OF SOMETHING THAT YOU'VE GOT ON YOUR DRAWING BOARDS THAT COULD BE REACTIVE IN TEN YEARS?
Not really. What we're really starting to do is build 'he building blocks. So, we're creating the Lego bricks. It's up to somebody else who understands, "Hey, these are Lego bricks. I can build really interesting stuff with them.' But we're going to have something that interlocks, that are all going to work together. That's an important first step.

THE RANGE OF POSSIBILITIES IS EVERYTHING FROM BEING ABLE TO COAT AN ENTIRE WALL TO BECOME A DIGITAL SCREEN OR CREATE A DRESS THAT HAD SMART THREADS WHICH COULD ACTUALLY CHANGE THE COLORS?
Or create a new pattern, even. Exactly.

WHAT ABOUT MEDICAL APPLICATIONS OF MOLECULE SIZE INTEGRATED CIRCUITS?
They could be diagnostics because these machines are smaller than a bacteria. So, you can imagine one of these up against a bacteria saying, 'Hey, this is a particularly bad strain.' And identifying it so the doctor knows how to treat it.

ANY POSSIBILITY THAT THESE KINDS OF INTEGRATED CIRCUITS COULD BE INSERTED INTO CANCER CELLS TO DEFEAT THEM?
It's a possibility. There's a huge number of other technical challenges, but if you could tell the cancerous cell from the non-cancerous cell that's clearly a tool you would like to have around.

THE PROGRAMMED INTEGRATED CIRCUIT ITSELF COULD EXPLORE THE BODY LOOKING FOR THE CANCEROUS CELLS.
Potentially. There's a lot of technical difficulties. For example, if you put anything in the body, the body quickly attacks it and eats it and destroys it.

BUT YOU'RE TALKING ABOUT THINGS MADE OUT OF CARBON.
The body attacks things made out of carbon. Our bodies are pretty smart. But nonetheless, in spite of the challenges, this is clearly going to be a tool of great interest to biomedical scientists.

WHAT DO YOU EXPECT TO BE THE FIRST FUNCTIONING PRODUCT?
In two years, we'll have something in the lab with very painstakingly difficult wires attached to it to prove that it's working. Only in the lab. Then, the baby will grow up. And in 10 years, I think there is a good chance that it could start competing head to head with existing integrated circuits in a lot of stuff.

That's around the time in 2010 when light or x-ray produced integrated circuits are going to find it pretty hard going because they won't be able to be made any smaller. But my guess is that we will see things before that. We are literally able to store information in a way that it won't erase when you take the power off. It's non-volatile on a scale of molecules. So, you might imagine very interesting CD ROMS with tremendous capability before 2010. That's clearly one of the early things you start thinking about.

SO THIS PLASTIC MATERIAL THAT COULD FUNCTION AT THE MOLECULAR LEVEL WITH THE WIRES AND THE SWITCHES WOULD BE ABLE TO TAKE THE LIBRARY OF CONGRESS ONTO A CD?
Might very well be able to. I haven't done that calculation, but we will be able to have immense storage capability from this.

HAVE YOU GUYS BEEN TALKING TO INTEL? I'M THINKING THAT INTEL PENTIUM CHIPS WOULD EITHER BE RUNNING SCARED OR THEY WOULD BE TRYING TO BUY UP YOUR IDEAS.
Well, HP works with a lot of companies. Everyone in the industry is going to follow this kind of idea. We've worked successfully with Intel in the past. So I expect if our horse does well in the horse race, and this is very early technology, there are going to be a lot of opportunities to take advantage of it.

AT THIS POINT HEWLETT-PACKARD WOULD BE WANTING TO PUT ITSELF IN THE FOREFRONT OF INTEGRATED CIRCUITS AND ALL THE TRADITIONAL WORK IT HAS DONE?
We have a very basic technology. And it's going to take a lot of work and different people in a lot of companies to understand the full business applications of this. We just want to be in a position to be one of the leaders.

IT' IS AS IF YOU ARE DESCRIBING A WORLD SO STRANGE THAT IT'S ALMOST BEYOND SCIENCE FICTION AS STRANGE IN 1999 AS THIS YEAR WOULD BE TO PEOPLE A HUNDRED YEARS AGO IN

THE YEAR 1899. COLLAPSING IN TEN YEARS WHAT TOOK A HUNDRED BEFORE.
I'm not sure it's 100 years to ten, but things are collapsing faster now. That is definitely true. And so, it's really important for the general public to hear about these things. To understand what potentially is coming.

Who would have guessed if you had been looking in the 1960s and 1950s and 40s and 70s even at movies that the invention of videotape would go to the MTV style of a video with its rapid jumping around. A very different style from movie making. And indeed, fashion might dramatically change to a very different style that anyone walking around today would ever expect. Stranger things have happened.

IT' IS SOMETHING TO REALIZE THAT WHAT WE'RE MOVING INTO IS A NEW REVOLUTION IN WHICH THE COATINGS ON EVERYTHING COULD BE THE POWER, THE I-C, THE COLOR, LIGHTS THE VERY COATINGS THEMSELVES.
Yes, it could be the coatings and the material it's made of, yes. One way of thinking about this - and I think potentially it is a new Industrial Revolution - is that we build these things very simply using chemistry. But then in affect, even if they have defects, we train them around the defects and produce very complex and very interesting things.

Right now, the I-C factories are so very expensive because they require a fortune in capital equipment to make very precise parts that fit together to make an I-C. We're saying, if you can build sloppy chemical parts, do it cheaply in a test tube. Even if they have defects, we're going to train around those defects using essentially smart labor of powerful supercomputers. So, computers are going to train this material to become smart. We're taking another step in the Industrial Revolution."

More Information:

1) Article: "Electronically Configurable Molecular-Based Logic Gates" *Science*, July 16, 1999, Pages 391-394.

2) For more information about another process to produce very small integrated circuits, see my Earthfiles.com report dated May 5, 1999, "Spinach Power for Integrated Circuits and Fuel Cells," in the science section.

Websites:

http://www.sciencemag.org

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