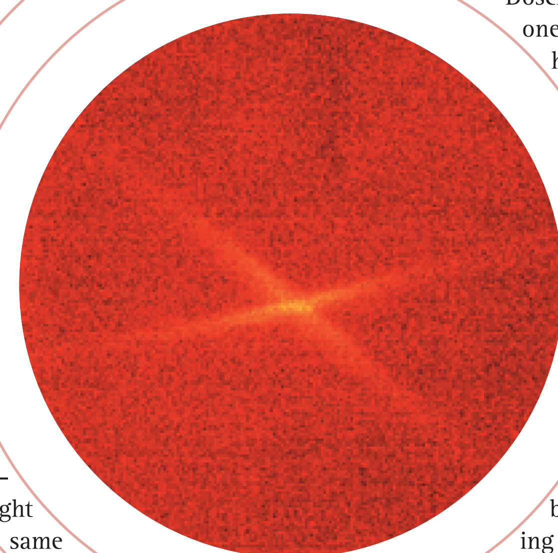
A digital **Machete** thins out the Data Jungle

"Around 98 percent of the stuff put out by computers is garbage which nobody reads". There is something in this claim attributed to an American news journalist. And who better to tell us a thing or two about it than all the physicists, chemists and astronomers who each day patiently, as if paralysed with fear, cope with the bulging output files of automatic measuring instruments.



One of these PC-stressed colleagues is Reinhard Streitel, who is tackling the surface properties of certain metal alloys in Helmut Dosch's study group at Stuttgart's Max Planck Institute for Metals Research. The young physicist sits at his desk in a small office in the Institute's new building in Stuttgart-Büsnau. Streitel pushes the computer's mouse back and forth amongst a handful of papers and pencils, types something on the keyboard, rummages through lists, then at last a video appears on the second screen: what we see is a kind of round window on which very gradually a sort of luminous reflectance begins to emerge resembling a blurred diagonal cross formed by two jets of flame against an orange, slightly out-of-focus background.

"Those are X-ray reflections, the result of time-resolved X-ray diffraction measurements we are using to study how the surface of a cobalt-gallium alloy changes in an oxygen atmosphere at high temperatures", explains Reinhard Streitel. Yet this, in itself simple, image is misleading: behind the apparently peaceful X-ray reflection lie huge data files – readings which Streitel takes with an X-ray detector in the atmosphere above the cobalt-gallium test specimen and has condensed into this video: it is like a digital iceberg with only a small percentage of the data visible. Streitel opens one of the files of "raw" detector data with an ASCII editor: over a megabyte of numbers, figures and data separators appears on the screen, an almost endless list of readings, only a fraction of which need to be processed to portray the reflection on the screen. In the past Reinhard Streitel and his colleagues used to extract from this jungle of symbols the data they actually needed laboriously, by hand so to speak or – if they were particularly smart – with a spreadsheet to prepare it for processing. It was a slow process.

In the past: that was before the American Kenneth A. Ritley joined the team of physicists – some eighteen months ago. "It became clear to me in just my first week here: I'm not extracting data laboriously by hand. What are computers for?" says Ritley. So he reached for his keyboard and developed a solution to the data problem.

Change of location. A somewhat larger, bright office in the same building. Helmut Dosch takes a blank sheet of paper from a pile and begins to draw. A diagram: a line, a surface with short lines bearing small semicircles at their upper ends arranged vertically along it. Dosch heads a department at Stuttgart's Max Planck Institute for Metals Research and also holds a chair at the Institute for Theoretical and Applied Physics at Stuttgart University – and he is interested in metastable and low dimensional material systems, in interfaces. Why are interfaces so interesting? "Because interactions between things inevitably always take place on their surfaces," says Dosch. "Think of corrosion, of heterogenous catalysis or just of friction between two metal surfaces. If you modify the surfaces, you can give them completely new properties with astonishingly little effort."

Materials scientists now have extremely complex apparatus in their tool boxes for doing just this: today, to quote an extreme case, one single layer of tailor-made molecules is enough to make copper water-repellent like a Teflon coating, for example, or to make the human body believe that the surface of an implant is organic in origin.

Dosch puts his pen to one side and explains his sketch: the short lines with the semicircles are molecules which are anchored to a surface. "We physicists are caricaturists. Complicated molecules fill us with horror. We try to make everything as simple as possible", he says, opening an article in a topical scientific magazine. "Molecules like this, for example." Dosch points to the ball and stick model of an enzyme. "Imagine that because of its shape this enzyme could identify sugar molecules and, as a result, emit electrons. If this enzyme were linked to a conductive surface by a flexible connection, tiny sugar sensors could be built with it which could even be implanted in blood vessels."

Alkane thiols provide another example: vaguely rod-shaped molecules which contain a sulphurous SH-group at one end – a functional group which bonds strongly with gold surfaces. Gold surfaces can be given virtually any property with this kind of combination, depending on how the end of the molecule furthest from the sulphur is constructed. For the alkane thiols are arranged on the gold surface like stalks of wheat: the SH group is the "root", the ear being the other end of the molecule. In the alkane thiol wheat field therefore the ears form a new surface with quite different properties. Viewed from the air, a wheat field looks quite different from a ploughed field – this is a poor comparison though, as the molecule layer, only a few angströms thick, is transparent and so not visible.

Research is in its infancy

If a water-repellent molecular component is inserted as the ear, then you get a gold film which water rolls off. If alkane thiols with more complex molecule groups are used as "ears", which bond to cholesterol molecules, the gold foil coated in this way can literally comb cholesterol out of solutions which can subsequently be identified using spectroscopy – and there you have a highly sensitive cholesterol sensor. "The possibilities are endless," says Dosch, "research in this field is still in its infancy."

At least as far as use of the arsenal of methods available to organic chemists goes: the materials scientists have only recently unlocked this huge tool cabinet which held the alkane thiols. Until now, surface coating was predominantly the playground of inorganic chemists who bombarded ceramic substrates with ions, for example, to produce semiconductor layers. "But organic molecules offer far greater creative latitude: they can be customised virtually at will for specific tasks. Moreover, they can be applied under much less rigorous conditions – if I dip gold foil in an alkane thiol solution, the coating is finished in principle," explains Helmut Dosch.

Yet the new opportunities are still giving Dosch's colleagues a few headaches: the chemists are currently working on increasingly complex "ears" and receptor molecules although we still do not know much about the laws which govern how these molecules are organised on surfaces, how they form structures and, for example, reorganise if exposed to high temperatures. For the desired, to a certain extent, two-dimensional crystalline arrangement of the molecular wheat field does not just develop of its own accord: molecules arrive from the wrong direction and must first find their place on the interface; this produces arrangements which may not necessarily resemble the "finished" structures. Scientists know, for example, that, at low levels of surface coverage, alkane thiols first organise themselves into structures which resemble a cornfield flattened by a hurricane; only as more and more of these rod-like molecules are brought to the gold surface do the stalks stand up straight. In other combina-

PHOTOS AND FIG.: MPI FOR METALS RESEARCH

How particles are arranged on surfaces: organic molecules (alkane thiols) on a gold surface. The diagram on the right shows the potential landscape.

Ultra-high vacuum chambers like this one are the centre of activity for Helmut Dosch's study group. In the chambers thin films are bombarded with molecules and irradiated with X-ray light.

tions with a multi-layer system, the arrangement of the upper layer may differ from that of the lower.

"We also observe a strong dynamic effect here: the molecules are mobile, that means, depending on the temperature they sit tight or move relatively quickly over the surface, disperse at random, arrange themselves into islands or form two-dimensional phases with domains running in different directions", says Dosch. Dosch currently uses relatively simply built model molecules to determine the timetable by which individual molecules cover free surfaces: flat disk-shaped polycycles, for example, resembling a small section of graphite's lattice plane, can quickly be converted however with slight modifications into chemical specialists similar to our old friends the alkane thiols.

But there is a catch: establishing how the particles organise themselves on the substrate is not an easy task. Computers are not much help. "The interactions between substrate and covering molecules are too complex for them", says Dosch. But how do you examine surfaces which only make up a tiny part of the test specimen? Any method which examines the sample against light has to be ruled out in advance. The molecule arrangement making up the interface is much too thin for that. Examining the sample under a microscope however would only provide a static image of the situation which tells us nothing about the dynamics of adsorption and self-organisation – to understand how a molecule film grows, the researchers must be able to actually look at the teeming mass on the surface in real time.

Dosch reaches for his pen again. He sketches a neon sign made from a thick sheet of plexiglass whose edge is illuminated by a hidden light source. Dosch explains: "If you look at right angles to the light directed at the sheet, you can't see that it is illuminated. But if you write on the sheet with a felt pen, the writing lights up." What is happening here?

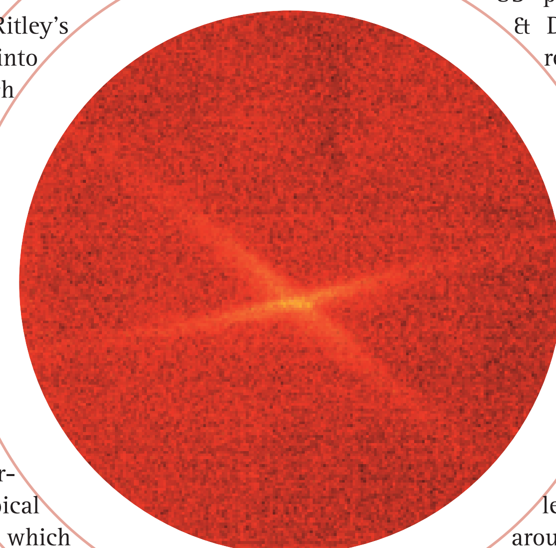
A FILM OF EVANESCENT WAVES

Evanescent waves provide the solution to the puzzle. Helmut Dosch draws detailed sections of surfaces: optical densities, light rays, refraction indices, total reflection. "If you irradiate a surface with light from a very shallow angle so that total reflection occurs, a film of light just a few micrometres thick develops at the interface. This film is made up of standing, so called evanescent ("vanishing") waves. The film of light can only be identified if these standing waves are disturbed by foreign bodies, such as particles of dust or pigment. The light is then scattered – and is visible to the observer."

Dosch makes use of this effect in his laboratory: he illuminates a surface on which organic or inorganic molecules are adsorbed with very intense X-ray light from a very shallow angle. Below certain angles total reflection occurs here too – and a thin film of invisible X-ray light, an evanescent X-ray light wave, also develops here immediately next to the interface. The trick: this wave is disturbed by the adsorbed molecules. Conclusions as to the arrangement and structure of the adsorbed molecules, even down to atomic details of the molecular structure, can be drawn from the distribution of the scattered X-rays.

However, the flood of data produced when X-ray reflections over the substrate surface are recorded is similar to that arising in structural chemistry laboratories when the only way to explain the atomic structure of complicated molecules is by X-ray crystal analysis: this mass of numbers makes real time analysis of organisational processes on the surface of a metal alloy really awkward.

This is where Ritley's solution comes into play. As Dosch says, "Kenneth has written a program which saves him converting the data he needs. No big deal really. To be honest, the success of this program has taken us quite by surprise. It's a typical case of a spin-off which from time to time achieves more than the actual main operation for which the program was created." ScanRead – the name given to the tool written in Visual Basic – actually does nothing more than remove unnecessary data from the gigantic spec files supplied by the detectors in Dosch's X-ray image cabinet and tidy them up so they can be understood by a commercial Windows data analysis program. "It didn't actually take much more than a week to write the routine", says Kenneth A. Ritley.



Yet, small effort – big result. Through ScanRead the Max Planck researchers in Stuttgart are now able to track on screen changes occurring in the surface structure of a substrate, adsorption and oxidation processes, for example, virtually the second they happen.

The surprise came for Dosch and Ritley when the postdoctoral researcher made his program available on the internet as a free download: within a short time a thousand copies of his software were making their way around the world, colleagues reached for the phone, technical journals like the renowned US publication Research & Development carried reports on the useful tool. "It shows that lots of people had a need for such a routine but no-one had taken the trouble to develop a programme like this themselves", says Ritley.

Encouraged by requests from colleagues – at the peak, around one a week – Ritley refined his program further. From a digital machete for clearing the data jungle it has now become a kind of Swiss army knife for physicists, which now not only clears out rampant lists of data regardless where they come from but also supplies a number of regularly needed arithmetical routines at the touch of a button: which all goes to show that major problems can be solved with minimal effort.

"We wondered whether to patent ScanRead but it didn't seem worthwhile", says Kenneth A. Ritley – a misjudgement. So Ritley's brainwave has not made his fortune although it has resulted in some degree of commercial success – although not quite as expected: in January of this year a well-known Sindelfingen IT company rolled out the red carpet for Ritley. "Ultimately, it was the idea of ScanRead rather than my physics research which was responsible for my appointment", says Ritley. Now the former physicist is making sure that the numerous different data streams within large companies will soon be flowing through a common channel – a task which looks suspiciously like the one Ritley has already mastered once.

COBALT OXIDE CRYSTALS GROWING IN A VACUUM

The other side of the coin: Dosch now has one outstanding man less on board. "That's how it goes", he says, "we're a hothouse for high-fliers." As he says this, Richard Streitel clicks on the ScanRead window on one of his screens. In the vacuum chamber cobalt oxide crystals are growing on a shiny silvery metal disk made from his cobalt-gallium alloy. Streitel points to the streaks which cross and shimmer on his screen. "These X-ray reflections here are produced by longitudinal cobalt oxide crystals which gradually form on the surface when the temperature exceeds 300 degrees centigrade." Streitel opens his degree dissertation: it contains microscope photos of these oxide surfaces which look like aerial photos of a city with "streets" running at right angles to one another and rectangular "buildings" of different sizes. Oxide films like this are important for the manufacture of magnetic storage media. Streitel clicks on one of the buttons in the ScanRead window. In a second the intensity profile of an X-ray reflection appears on the second screen. Then another. And another. Within a second. As simple as that.

STEFAN ALBUS

SINDELFINGEN IN PLACE OF SILICON VALLEY

Dr. Kenneth A. Ritley is an American "IT recruit": After a postdoctoral period with Helmut Dosch's study group at Stuttgart's Max Planck Institute for Metals Research, he didn't pack his bags to continue his career in the States but stayed in Germany – thanks to a green card and an unlimited residence permit which Ritley's new employer, Sindelfingen's HP Consulting, obtained in record time. Why does someone who can choose between Silicon Valley and Sindelfingen stay in Germany? Is Germany perhaps not as bad as we think?

MPF: *Dr. Ritley, you have every opportunity open to you in your own country. Why are you staying here?*

RITLEY: It's true you can soon earn a lot of money in America if your work's good. But the quality of life is higher in Germany.

MPF: *How do you mean?*

RITLEY: I like skiing, for example –the conditions are obviously ideal here (smiles). Of course, that's not the only thing. In America I only get one week's holiday, for example – here it's 48 days. Also I'll be getting a company car here soon, I'd have to wait a lot longer in America. And I have to say: I like Germany. My experience over here has been good. For example, it was marvellous working with Helmut Dosch. The atmosphere within his group is outstanding, right from the start he let me do the work I wanted to do. I don't know if Helmut is a typical German though.

MPF: *He's more like we imagine the Americans. But isn't IT much more advanced in America? Aren't the opportunities over there quite different?*

RITLEY: True –the IT industry positively took off in America five years ago. That's just happening in Germany now. For example, HP Consulting took on 300 new staff last year – and it could have been far more. If our workforce was ten times bigger, we could work on ten times as many contracts. There's more work than we can deal with. But this awakening is precisely the attraction: I can be involved here right from the start and help shape development.

MPF: *German is supposed to be difficult. Is the language a problem for you?*

RITLEY: Yes. At HP we speak High German. In Helmut Dosch's group I tended to learn the Schwäbisch dialect. But I'm getting the hang of it.

INTERVIEW BY STEFAN ALBUS.