Writing a Scientific Paper: One, Ideosyncratic, View

George M. Whitesides

Department of Chemistry and Chemical Biology

Harvard University

gwhitesides@gmwgroup.harvard.edu

231st ACS National Meeting, Atlanta, GA, March 26-30, 2006
Division of Chemical Information, CINF-17

- Writing is/should be an integral part of research, not a separate activity
- It is efficient to focus research on getting the information needed for the paper, rather than on wandering randomly in intellectual phase space.

- *Do NOT do the research, then write the paper! Use the writing to manage the research.*

In science, one writes for many audiences

- Peers/editors, for peer-reviewed journals
  - Different fields/people/journals are different
- General audiences, for whom TV is always an alternative
  - Scientific American
  - Popular writing
  - Newspaper
- Faceless bureaucrats, for government reports (NRC, …)
- Hostile, skeptical, or indifferent referees, for proposals and reports
- ….and so on

Prose for a scientific paper

“We present a top-down technique that generates patterned arrays of gold nanowires of uniform, controllable length, width, and height, and describe a systematic study of the dependence of the surface plasmon resonance on the geometry of these wires. This fabrication technique combines photolithography, thin-film metal deposition, and thin-film sectioning. The cross-section of these nanowires is determined by the thickness of the deposited metal film, and by the thickness generated by sectioning, and can be as small as 10 nm × 30 nm. The surface plasmon resonance of individual wires is determined by the geometry and size of their cross-sections. The plasmon resonance peak of a given nanowire shows a red shift with the increase of the aspect ratio of its cross-section, in agreement with simulations based on the Finite-Difference Time-Domain method.”

(Prepared for, and rejected by, *Nature.*)

Prose for a coffee-table book

We know "now";

we remember "then."

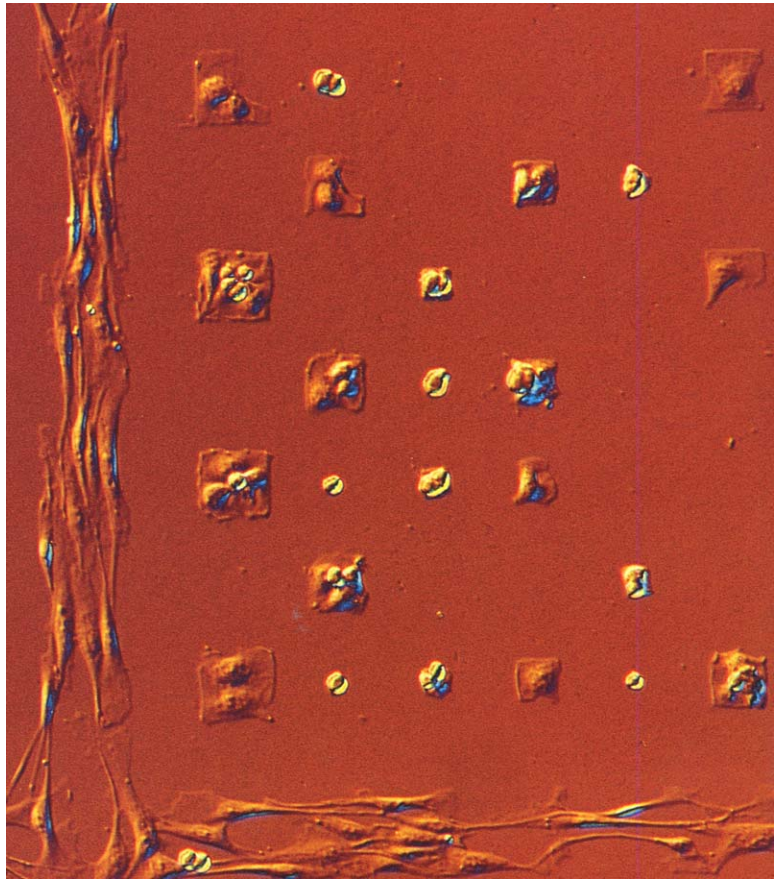
If the two are different,

that is change.

We are immersed in a world of clocks. All that happens meters time. The universe expands, continents collide, we age, leaves change color, the sun sets, children play, we breathe, the wind rustles in the grass.

mammalian cells on a patterned surface

We avoid death. We think of it as an undesirable accident in the plumbing: an artery clogs or bursts; a tumor pushes the machinery out of line; an automobile at the wrong time and place reduces us to mush. Still, proper maintenance forestalls the inevitable, and we are emotionally disposed to live forever.



"On the Surface of Things" Frankel and Whitesides

Prose for a government Report

SUMMARY OF RECOMMENDATIONS TO THE DOD

1. ACCEPT THAT THE POTENTIAL OF SOPHISTICATED BIOLOGICAL ATTACK IS COMPARABLE TO THAT OF NUCLEAR ATTACK IN ITS POTENTIAL TO CAUSE CASUALTIES AND DISRUPT SOCIETY.

2. FIRST, PROTECT YOUR OWN: BY ENABLING THE MILITARY MISSION, YOU STRENGTHEN CIVILIAN DEFENSE.

3. IMPLEMENT A COHERENT STRATEGY FOR BIODEFENSE AND PUT SOMEONE IN CHARGE.

4. ANTICIPATE A CENTRAL ROLE IN CIVIL SUPPORT.

5. BUILD A STRONG SCIENCE AND TECHNOLOGY BASE FOR BIOLOGICAL DEFENSE.

6. AVOID SURPRISE: REENGINEER THE ROLE OF INTELLIGENCE IN WARNING AND DETERRENCE.

7. EDUCATE, GAME, RED-TEAM, EXPERIMENT, EXERCISE, AND TRAIN.

GENERATING A ROBUST DEFENSE REQUIRES ELEVATING THE PRIORITY OF BIODEFENSE IN THE DOD AND NATIONALLY. IT ALSO REQUIRES COMMITTING TO A SUSTAINED PROGRAM IN SCIENCE AND TECHNOLOGY TO BUILD AND INTEGRATE THE COMPONENTS THAT ARE REQUIRED FOR A CAPABILITY SUFFICIENTLY STRONG TO DETER THEIR DEVELOPMENT AND USE.

CHAPTER 2 SUMMARY OF FINDINGS

The subject of biological defense is a complicated one, with aspects that include threat assessment, assessment of defense capability, technology for defense, organization, leadership, and policy. This chapter summarizes the major findings of the DSB/TRAC Task Force: analysis supporting these findings is detailed in Appendix II.

SITUATIONAL ASSESSMENT

1. Biological weapons pose a very serious threat to the U.S., its armed forces, its civilian population, and its allies. Plausible biological attacks today can make it difficult or impossible to conduct military operations. The application of widely available techniques of biotechnology in the future will make this threat yet more serious.

2. The capability to defend both military and civilian targets is essential to national security.

3. Biodefense mixes national security, public health, consequence management, and law enforcement; integrating these four sectors to build a defensive capability poses a major organizational challenge.

4. For many plausible types of biological attacks (especially on civilian targets), there will be no warning. The assumption that appropriate sensors, by themselves, will provide a high level of protection is unfounded. The ability to manage the consequences of a consummated attack is a *required* component of biodefense.

5. It is not possible to quantify the risk of a high-level biological attack. It is much like a nuclear strike—very low probability, but extremely high consequences. The technical capability to carry out such an attack exists and will improve with time; motivation and intent cannot be assessed accurately.

Writing the paper should be an integral part of research, not a separate activity

- **As soon as there is *real* result, make an outline**
- **Refine the outline drafts, and paper drafts, as research continues**
- **Tentative outline → Outline → Working paper → Submitted manuscript is a continuous process.**
- **Focus the research on getting the information needed for the paper.**
- ***Do NOT do the research, then write the paper!***

Most experimental papers in science follow a template

- **Title**
- **Authors**
- **(Abstract: *for abstracting services*)**
- **Introduction: *Crucial in understanding "why?"***
- **(Experimental Design)**
- **Results and Discussion**
- **Conclusions**
- **Experimental Section**
- **(Acknowledgments)**
- **References**
- **Supplemental Material: *More and more of the paper***

- eTransport in Organic Materials
- Objective: New function
- Organic electronics: OLEDs, memory, microprocessors
- Molecular electronics: the hope for very small processing units
- (e.g., molecules), perhaps with new function (defined by IV response)
- Boundary conditions: ultimately should be something that one can use
- in devices (memory, microprocessors, displays, sensors, actuators)
- Current State
- No solid body of theory to use in building materials
- Interfaces; 1D vs 3D;
- Substantial uncertainty about reproducibility of many data in
- molecular electronics
- History
- Justification
- "end of Moore's Law"
- Low-cost electronics
- Fundamental: physics of eT
- Organics offer the potential of much more detailed engineering
- of electronic structure than semiconductors
- Two different threads
- OLEDs: major progress
- Electronics: Initial excitement, but very little of the work
- has been reproduced, and much is believed to be irreproducible
- What is the problem?
- Conclusions to date:
- Tunneling
- Hole transport
- Open Questions
- Are there unusual/useful effects?
- What is the mechanism/s of eT?
- How to think about hole transport
- Can one design organic matter to give desired effects?
- New Tools
- Conventional
- STM, junctions fabricated by standard Si microfab technology
- New
- Our focus: Hg drop and SAMs
- Characteristics
- Plusses and minuses
- Others
- Hg drop in siloxanes on Si
- What else?
- Our Results
- Tunneling
- Role of Defects
- Influence of Structure: R2S vs RSH; Different metals--no unusual
- effects: SAMs are a layer of "fat"
- Metrology: beta; J
- Your work on colloids?
- Effects reported in the literature
- Future
- SAMs are models; Colloids? Stable organometallics?
- Upper junction

Outlines:

Just Scribble it down!

First: ideas

Then: organization

Outlines

Title: ELECTRON TRANSPORT IN MONOLAYER FILMS OF ORGANIC MOLECULES

INTRODUCTION

Objective: New function

Organic electronics: OLEDs, memory, microprocessors

Molecular electronics: the hope for very small processing units (e.g., molecules), perhaps with new function (defined by IV response)

Boundary conditions:

Ultimately should be something that one can use in devices (memory, microprocessors, displays, sensors, actuators)

Current State of field

No solid body of theory to use in building materials

Interfaces; 1D vs 3D;

Substantial uncertainty about reproducibility of many data in molecular electronics

Early-Stage Outline:

Objective: Agreeing on structure and content.

- AFM Studies on Crack Morphology
  - Figure 2 shows the AFM images of cracked Si. (A) The surface scan and cross section of a crack ~ 0.5 mm from the crack tip. The cross-section shows a step height of ~ 5 nm. (B) The surface scan and cross section of the same crack ~ 0.1 mm from the crack tip. The cross-section shows a step height of ~ 1 nm. (C) The surface scan and cross section for the same crack at the crack tip near the limit of detection, step height ~ 0.1 nm.
  - It is important to note that ~~this~~ is a step, not a nanogap. This suggests that the cracking of silicon wafer is the result of a mechanical twist of two crystal planes. The slope of the twist~~ed~~ crystal planes of this sample shown here is ~~quite~~ small (S ≈ 1 nm/100 μm).
- Cracks and the Limits of Replica Molding
  - Figure 3 shows the AFM images of a PDMS replica of the same silicon crack shown in Figure 2. (A) The surface scan and cross section for the sample ~ 0.5 mm from the crack tip, with step height of ~ 5 nm. (B) The surface scan and cross section for the sample ~ 0.1 mm from the crack tip, with step height of ~ 1 nm. (C) The surface scan and cross section for the sample near the tip of the crack. We can see a faint line in the AFM area scan that corresponds to the crack, but we cannot see the height difference in a single cross-section since the roughness of the PDMS surface is ~0.5 nm to 1 nm (larger than the crack itself).

Middle-Stage Outline/paper

Objective: Getting the science right -- *efficiently!*

control. ~~Once fractured, the wafer must always be stabilized with a second back-layer to prevent propagation of the crack during replica molding or other manipulations.~~ ~~Figure~~ 1b describes the molding process ~~schematically~~. We ~~demonstrate~~ transfer ~~of~~ the relief structure of the crack, sequentially, to two different polymers: ~~an elastomeric poly(dimethylsiloxane) (PDMS) stamp, and a hard, UV-curable polyurethane (PU) replica.~~ The replication process was accomplished in three steps: 1) generation of the silicon crack; 2) fabrication of an elastomeric stamp ~~from the crack with~~ a composite stamp comprising a ~100-μm layer of ~~"hard" poly(dimethylsiloxane)~~ (*h*-PDMS) in direct contact with the surface, and a ~2-mm thick layer of "soft"-poly(dimethylsiloxane) (*s*-PDMS) as a backlayer;[11-13] 3) replication of the crack relief structure ~~into polyurethane~~ (PU) ~~using~~ the PDMS stamp.

Figure 2A shows the AFM image of the tip of a crack in silicon. ~~It is important to note that~~ within 100 μm of the tip, there is no gap ~~where~~ the two Si planes ~~meet~~. This observation ~~indicates~~ that the crack ~~was formed~~ by a slip-dislocation along a [100] plane, rather than in-plane separation of the silicon along the crack. The dashed lines in the figure indicate locations along the crack ~~for~~ which ~~cross-sections are displayed~~. For this crack, ~~a point of inflection (kink)~~ close to the tip provided a point of reference for comparison between master, mold, and replica.

Figure 2B shows the AFM image of the replicated crack in PDMS. The original image has been flipped horizontally and the color has been inverted so that the replica can be directly compared to the master. The absence of an upraised spike along the ridge of the crack indicates that there is minimal penetration of the PDMS pre-polymer between the Si planes (i.e. there is no gap between the planes). We attribute the bright

Late-Stage Paper

Objective: getting the prose and presentation of data right

scribe. The applied pressure was vertical to the plane of the wafer. The crack propagated only to the vicinity of the boundary defined by the glass backlayer; thus, the length of the crack could be controlled to within a few mm by the position of the glass slide. After cracking the wafer, we bonded a second glass slide to the backside of the cracked region with epoxy; this slide froze the crack, and prevented further growth. Fractured Si, stabilized by binding to a glass backlayer, is remarkably robust and can, for example, withstand spin-speeds in excess of 2000 rpm without noticeable crack propagation.

We transferred the relief structure of the crack, sequentially, to two different polymers using techniques described previously for soft lithography (Fig. 1B).[4] The replication process was accomplished in three steps: 1) generation of the crack in silicon; 2) fabrication of a composite elastomeric stamp using the cracked wafer as a master, ~~and formation of a~~ composite stamp comprising a ~100-μm layer of *h*-PDMS in direct contact with the surface, and a ~2-mm thick layer of "soft"-poly(dimethylsiloxane) (*s*-PDMS) as a backlayer;[11-13] 3) second generation replication of the crack relief structure from the composite PDMS stamp using hard, UV-curable polyurethane (PU).

Fig. 2A shows the AFM image of the tip of a crack in silicon. Within 100 μm of the tip, there is no perceptible -- within the resolution of our AFM -- gap between the two Si planes. This observation suggests that the crack forms by a slip-dislocation along a (100) plane, rather than in-plane separation of the silicon along the crack. The dashed lines in the figure indicate locations along the crack at which we measured surface profiles. For this crack, a kink in the crack close to the tip provided a point of reference for comparison between master, mold, and replica.

Graphics!

- “A picture is worth a thousand words” dramatically understates the opportunity.

Approaching Zero: Using Crystal Fractures to Generate Nanoscale Steps

Qiaobing Xu, Brian Mayers, George M. Whitesides*

IN	OUT
3/11/04	3/11/04
part in this date	3/30/04
4/30/04	5/1/04
05/10/04	5/12/04
8/26/04	8/28/04 -
09/20/04	9/22/04
09/27/04	9/29/04
10/06/04	10/10/04
Qiaobing date here → 10/21/04	10/21/04
10/22/04	10/22/04
10/26/04	10/30/04

The *Second* Task: Catching the Attention of a *Potential* Reader

- You have only the first two or three sentences to catch the attention of a reader. Don't waste them on generalities and background.
  - The title is crucial. ("How to make water run uphill")
  - The introductory paragraph is crucial
  - Good pictures are crucial
  - So, what about the rest of the paper?

- If you do the research, and write the paper, and no one reads it, why did you do it?

Introduction to The Introduction: The Saalfeld Criterion

- **Assume you have all the money you want, *and more***
- **Assume your research goes *better* than you could have expected**

- **Who cares?**
  - **Don't confuse "fundamental" and "useless"**

The Introduction

- **The first paragraph**
  1. **What you did: principal result**
  2. **Why you did it: motivation**
  3. **Who cares?: importance**
- **Statement of the problem**
- **Background and prior work**
  - **Be generous in acknowledging prior work. It's the right/ethical thing to do. Also, it was done by your referees!**
- **Your approach**
- **The principal result(s): *guide* the reader—it can be dangerous when people think for themselves.**

- **Experimental Design (?)**

Results and Discussion

- These are the scientific core, but they vary with the details of the research.
- "Short", "non-redundant", "grammatical", "clear", "explicit", "informative", are good adjectives.
- Put the most important results first.
- Leave out the history of your struggles.
- Shorter is always better.
- Make it short. Take out words.
- Short, short, short.
- Short. Clear.

Conclusions

- **The "conclusions" section is *not* an abstract. If you've said it once in the body of the paper, you don't have to say it again.**
- **It should put the work in context, and look at it from 30,000 ft**
  - **What? Why? Who cares? Why should they care?**
  - **Plusses and Minuses**
  - **Comparisons with other results/methods**
  - **Significance**
  - **Do you have a new perspective on the problem? (Use the active voice, and personal tone. "We believe that…" is useful if used in moderation.**

Grammar and Logic are Inseparable

Reference

- **Active voice: "We analyzed…", rather than "The data were analyzed…**
- **This (noun): "This demonstrated that…."**
- **Dependent clauses: "A and B and C and D, illustrating that …."**

If it is difficult to read, the reader stops reading.

It's all in Strunk and White, "The Elements of Style"

The three (or four) stages of a project

1. *(Identifying the problem)*
2. Defining the scientific problem
3. Solving the problem
4. Selling the solution

   If no one reads it, why bother to do it?

Will it all be different in the future?

- The “Supplemental” in peer-reviewed journals
- Electronic publishing
- The tsunami of information
- Google vs “the Book”
- Definition of problem → Research → Quality control → Dissemination/distribution → (Discovery)/Use
- Group/Mission Research vs Single-investigator/Peer Reviewed Research
- Blogging