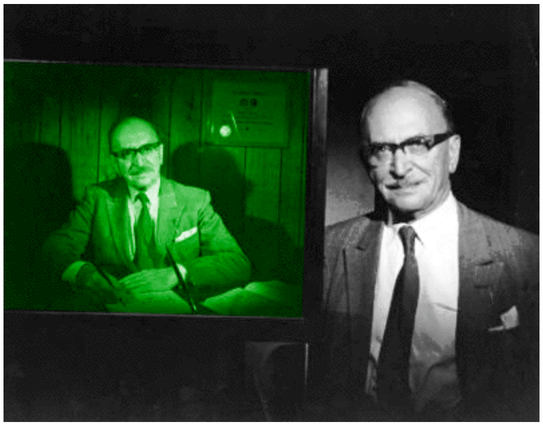
Holographic Images of Atoms: Past Achievements and Future Prospects



Dennis Gabor, 1971 Nobel Laureate in Physics

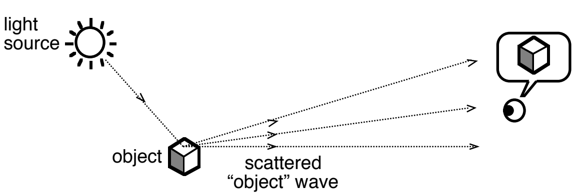
Patrick M. Len
Department of Science, Math and Engineering, Cosumnes River College
Department of Physics, University of California, Davis

Outline

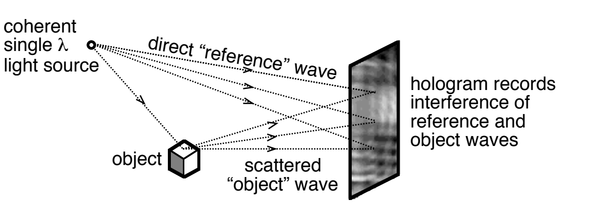
- Basic principles of holography
  - Encoding/decoding process
  - Optimal criteria for making holograms
  - Making atomic holograms
- Holographic images of atomic structure
  - Photoelectrons
  - X-rays
  - γ rays
  - Neutrons
- Advanced principles of atomic holography
  - Convolution/deconvolution process
  - Deconvolution kernels
- Conclusions:
  - Future prospects of atomic holography

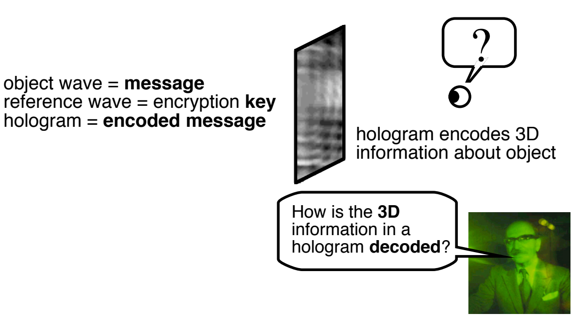
- Basic principles of holography
  - Encoding process

Light scattered from an **object** contains **3D** information

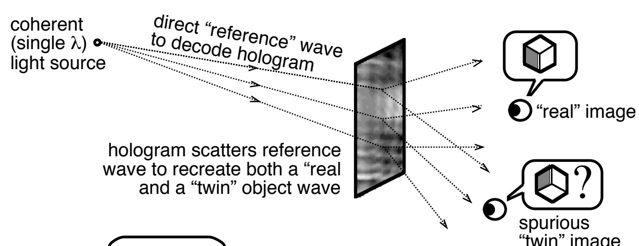


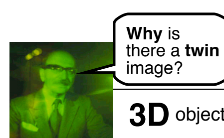
Light scattered from an object can be recorded, relative to a direct wave





- Basic principles of holography
  - Decoding process



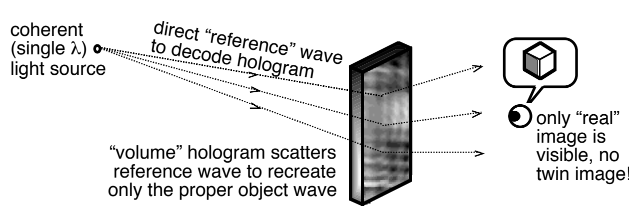


3D object→**2D** hologram→**3D** image (**real** *and* **twin**)

Ambiguity is introduced in **2D** encoding of **3D** information

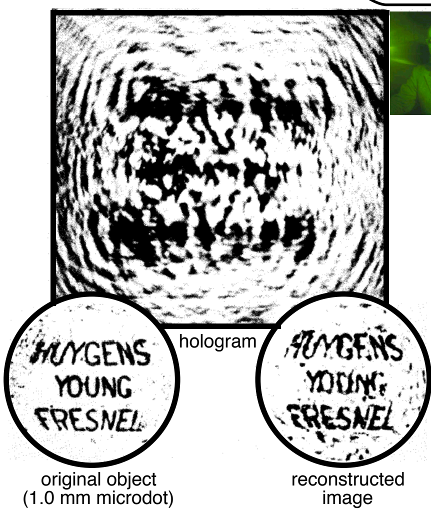
How to **suppress** twin images?
3D object→**3D** hologram→**3D** image (**real** only, **no** twin!)

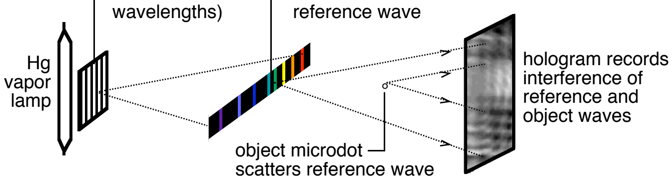
∴ record **2D** holographic data over a **third** parameter
(thick "volume" film emulsions, or for different λ values)



• Basic principles of holography
Gabor's original hologram

How was this done in **1947** without **lasers**?



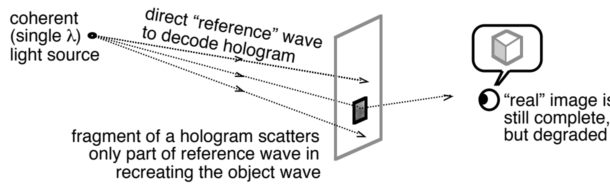


• Basic principles of holography
Optimal criteria for a "good" hologram

1. **Coherent reference wave source?**
   Ideal scattering by object
   "Well-behaved" waves required

2. **Small, specific λ wavelength value?**
   λ ≤ smallest resolvable details on object

3. **Sampling of large 3D hologram "volume"?**
   Suppresses twin images, artifacts, and improves image quality

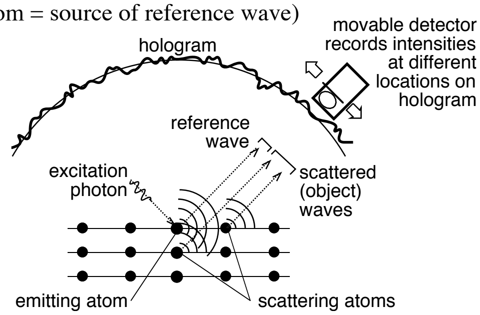


4. **Accurate recreation of reference wave**
   Important decryption step!

Can **atoms** make **holograms** of **themselves**?

• Basic principles of holography
Making atomic holograms

(a) inner source, outer detector
(atom = source of reference wave)



1. **Coherent reference wave source?**
   Ideal scattering by objects?
   Atom ≈ tiny source or scatterer of coherent photoelectrons, fluorescent x-rays, or γ rays, any of which will make holograms

2. **Small, specific λ wavelength value?**
   Photoelectron, fluorescent x-ray, or γ ray wavelength λ ≤ atomic spacing

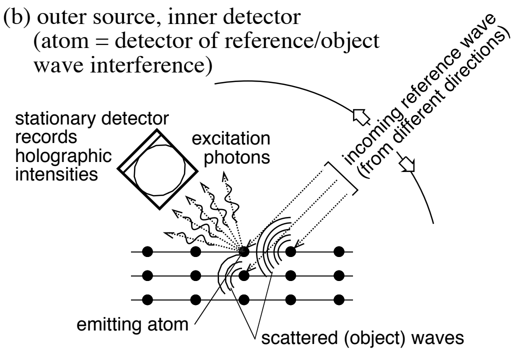
3. **Sampling of large 3D hologram "volume"?**
   Cannot change λ wavelengths of x-rays or γ rays emitted by an atom!

4. **Accurate recreation of reference wave?**
   To be done on a computer, rather than experimentally

What will happen to **images** from **single** λ holograms?

• Basic principles of holography
Making atomic holograms in reverse

(b) outer source, inner detector
(atom = detector of reference/object wave interference)



Interpretation:
"Backwards" case of "inner source, outer detector" holography
Holographic data is still the same as from before

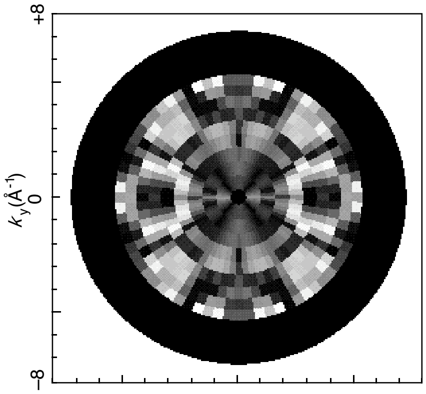
3. **Sampling of large 3D hologram "volume"?**
   Cannot change wavelengths of x-rays or γ rays emitted by an atom, but...

   "Third dimension" obtained by varying λ of **incoming** reference wave (electrons, x-rays, γ rays, neutrons)

   Twin images are suppressed!

Let's see the **holographic images of atoms**!

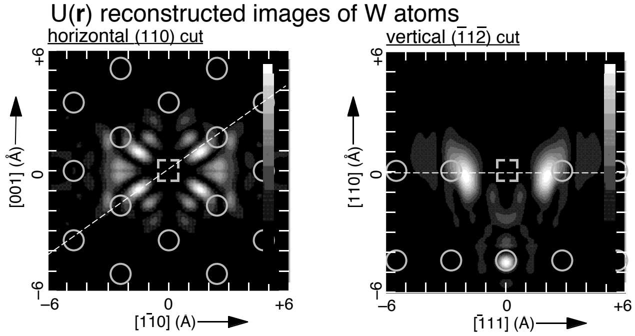
• Holographic images of W(110) surface
Photoelectrons emitted from surface atoms



$\chi(\mathbf{k})$
photoelectron
hologram
(top view)

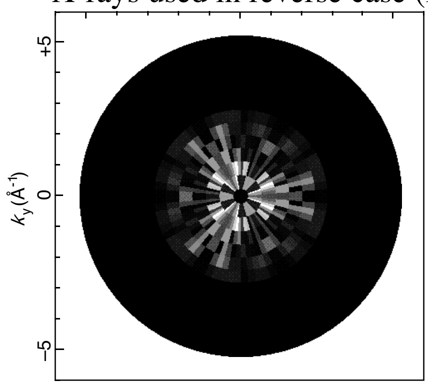
Delinger,
Rotenberg,
Len *et al.*, 1999

U(**r**) reconstructed images of W atoms



Strong scattering→data easy to collect
Complex, non-ideal reference/object waves→non-ideal images!

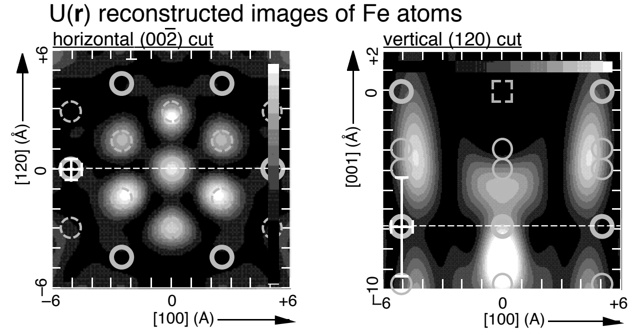
• Holographic images of hematite (Fe_2O_3)
X-rays used in reverse case (inner detector)



$\chi(\mathbf{k})$
fluorescent
x-ray
hologram
(top view)

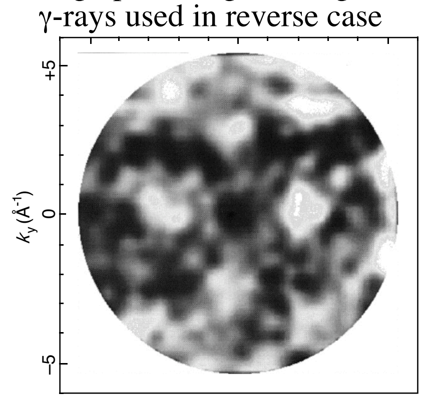
Gog, Len,
et al., 1996

U(**r**) reconstructed images of Fe atoms



Weak scattering→data not easy to collect
Heavier atoms scatter stronger than light atoms→only Fe visible
Simple, more ideal reference/object waves→better images!

• Holographic images of MgO
γ-rays used in reverse case

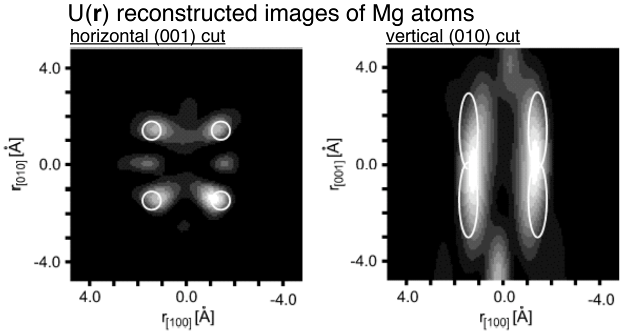


$\chi(\mathbf{k})$
γ-ray
hologram
(top view)

Korecki,
Korecki, and
Slezak, 1997

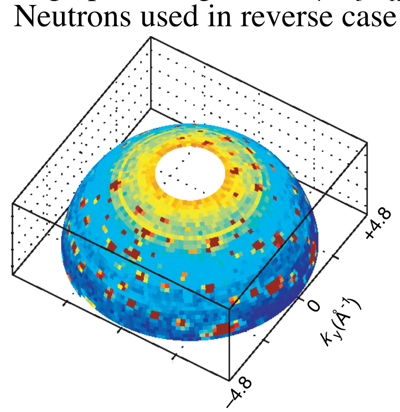
(First γ-ray
holography
experiment)

U(**r**) reconstructed images of Mg atoms



Simple, ideal reference/object waves→good images
Heavier nuclei scatter stronger than nuclei atoms→only Mg visible
Very small γ ray wavelengths→nuclei images!

• Holographic images of $Al_4Ta_3O_{13}(OH)$
Neutrons used in reverse case (inner detector)

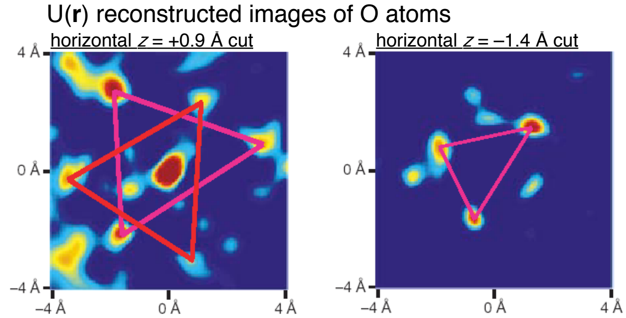


$\chi(\mathbf{k})$
neutron
hologram
(oblique view)

Sur *et al.*,
2001

(First neutron
holography
experiment)

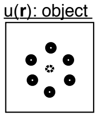
U(**r**) reconstructed images of O atoms



Simple, ideal reference/object waves→good images
Heavy/light nuclei scatter similarly→heavy and light nuclei visible
Neutron/nucleus spin scattering→spin holograms possible!

• Advanced principles of holography
Convolution/deconvolution process

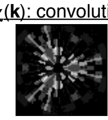
u(**r**): object



scattering "convolution" K(**k**,**r**)

$(\mathbf{r})^3 \longrightarrow (\mathbf{k})^3$

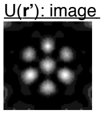
χ(**k**): convolution



A χ(**k**) **hologram** can be considered a **k**-space **convolution** of an **r**-space **object** u(**r**).

$$\chi(\mathbf{k}) = \iiint d^3\mathbf{r}\, \underbrace{K(\mathbf{k},\mathbf{r})}_{\text{convolution kernel}}\, u(\mathbf{r})$$

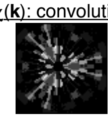
U(**r'**): image



reconstruction "deconvolution" κ(**k**,**r'**)

$(\mathbf{r}')^3 \longleftarrow (\mathbf{k})^3$

χ(**k**): convolution



The **object** can be reconstructed by properly **deconvoluting** the **k**-space hologram.

$$U(\mathbf{r}') = \iiint d^3\mathbf{k}\, \kappa^*(\mathbf{k},\mathbf{r}')\, \chi(\mathbf{k})$$

$$\propto \iiint d^3\mathbf{k}\, \kappa^*(\mathbf{k},\mathbf{r}') \iiint d^3\mathbf{r}\, K(\mathbf{k},\mathbf{r})\, u(\mathbf{r})$$

$$\propto \iiint d^3\mathbf{r}\, u(\mathbf{r}) \iiint d^3\mathbf{k}\, \kappa^*(\mathbf{k},\mathbf{r}')\, K(\mathbf{k},\mathbf{r})$$

orthogonality condition

$$\propto \iiint d^3\mathbf{r}\, u(\mathbf{r})\, \delta(\mathbf{r}-\mathbf{r}')$$

$$\propto u(\mathbf{r}')$$

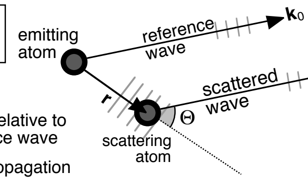
What do these K(**k**,**r**) and κ(**k**,**r'**) kernels look like?

• Advanced principles of holography
Convolution/deconvolution kernels

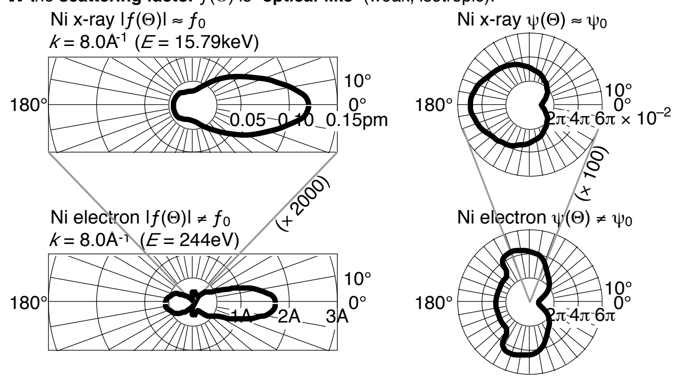
If the **convolution** K(**k**,**r**) can be modeled by a **single scattering** process:

$$K(\mathbf{k},\mathbf{r}) \propto f_k(\Theta)\, \frac{e^{-ikr}}{kr}\, e^{i\mathbf{k}\cdot\mathbf{r}}$$

- plane-wave scattering factor $= |f_k(\Theta)|\, e^{i\psi(\Theta)}$
- free-space propagation
- phase relative to reference wave



If the **scattering factor** ƒ(Θ) is "**optical-like**" (weak, isotropic):

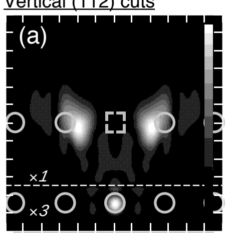


Then this **reconstruction kernel** κ(**k**,**r'**) will be **orthogonal** to K(**k**,**r**):

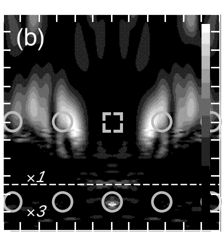
$$\kappa(\mathbf{k},\mathbf{r}') \propto e^{i(\mathbf{k}\cdot\mathbf{r}' - kr')} \Rightarrow \iiint d^3\mathbf{k}\, \kappa^*(\mathbf{k},\mathbf{r}')\, K(\mathbf{k},\mathbf{r}) \propto \delta(\mathbf{r}-\mathbf{r}')$$

How well does this **reconstruction kernel** work?

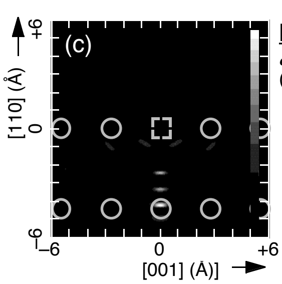
U(**r**) reconstructed images of W atoms
(Len, Denlinger, Rotenberg *et al.* 1999)
Vertical ($\bar{1}1\bar{2}$) cuts



Method (a):
modified kernel to deconvolute non-ideal single scattering
(Tonner *et al.*)



Method (b):
QM electron propagation kernel
(Lippman/Schwinger)



Method (c):
ad hoc orthogonal kernel
(Hoffman/Schindler, Woodruff)

What does an **improvement** in **image** quality say?

• Future prospects of atomic holography
Conclusions

Already done

Development of theory
Recognition of that atoms can create holograms of themselves

"Proof-of-principle" experiments
Holographic images obtained
(of atomic structures that were already known)

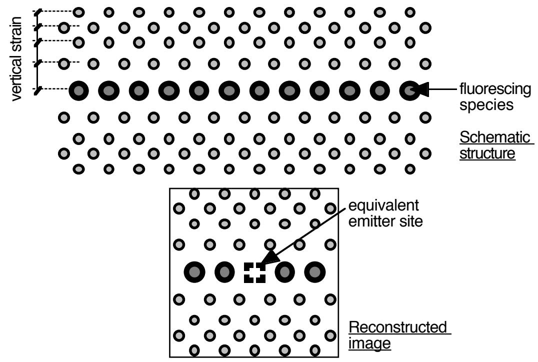
"You can't **predict** the **future**, but you can **invent** it."

Future prospects

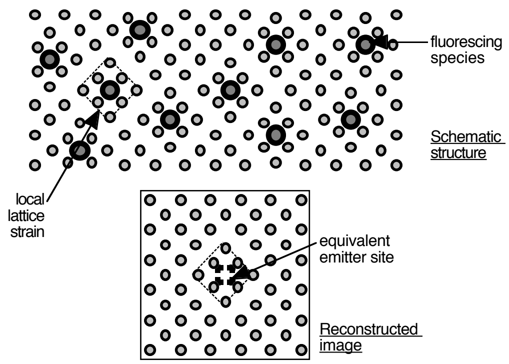
Improvement of theoretical understanding of electrons
- Using "bad images" of known structures to back-engineer scattering behavior at the atomic level
- Development of better reconstruction kernels and better understanding of electron scattering

Improvement of experimental techniques
- Faster/efficient detectors to record better holographic data for
  - x-rays
  - γ rays
  - neutrons
- Obtaining *a priori* holographic images of atomic structures (unknown/unobtainable/uncertain via conventional methods):
  - biomolecules
  - local structure of quasicrystals
  - other locally identical, but translationally disordered systems

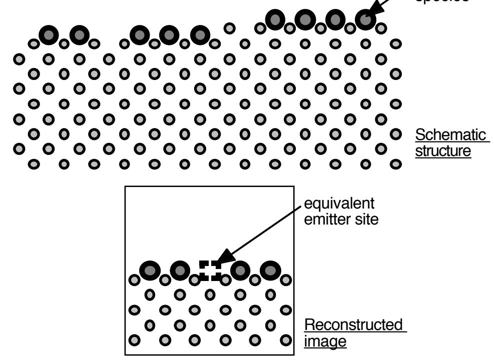
(c) Epitaxial δ-layers



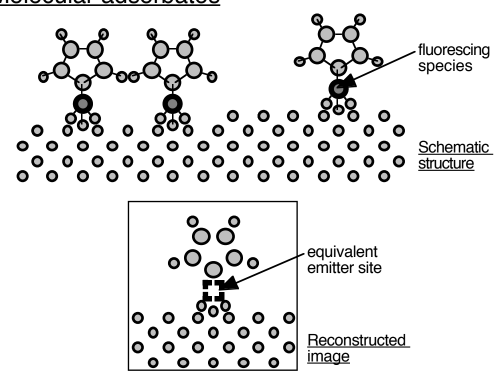
(d) Dopants



(e) Atomic adsorbates



(f) Molecular adsorbates



(g) Biological macromolecules