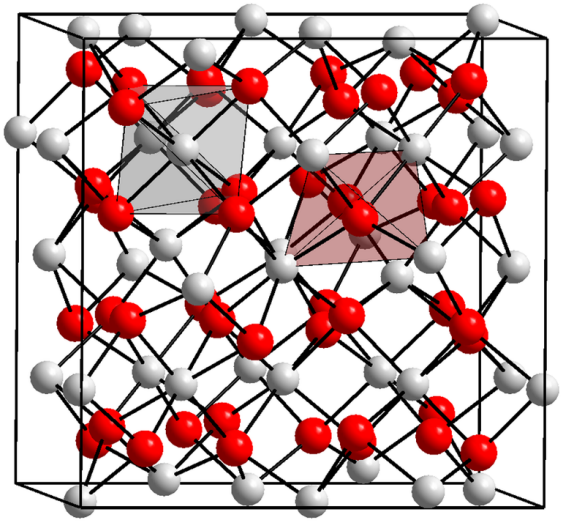
ITO

Indium tin oxide (ITO) is a ternary composition of indium, tin and oxygen in varying proportions. Depending on the oxygen content, it can either be described as a ceramic or alloy. Indium tin oxide is typically encountered as an oxygen saturated composition with a formulation of 74% In, 18% O2, and 8% Sn by weight. Oxygen saturated compositions are so typical, that unsaturated compositions are termed oxygen deficient ITO. It is transparent and colourless in thin layers while in bulk form it is yellowish to grey. In the infrared region of the spectrum it acts as a metal-like mirror.

Indium tin oxide is one of the most widely used transparent conducting oxides because of its two chief properties, its electrical conductivity and optical transparency, as well as the ease with which it can be deposited as a thin film. As with all transparent conducting films, a compromise must be made between conductivity and transparency, since increasing the thickness and increasing the concentration of charge carriers will increase the material's conductivity, but decrease its transparency.

Thin films of indium tin oxide are most commonly deposited on surfaces by physical vapor deposition. Often used is electron beam evaporation, or a range of sputter deposition techniques.



Crystal structure: Cubic, space group Ia3 No. 206, cI80, a = 1.0117 nm, Z = 16

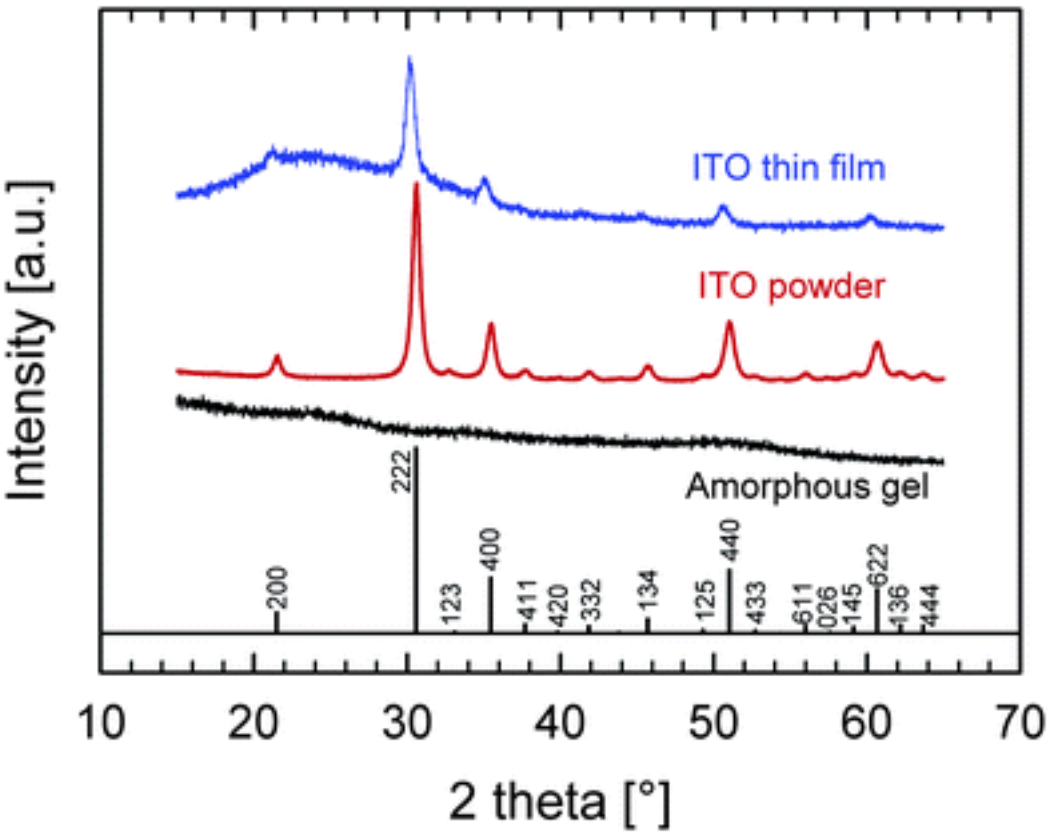


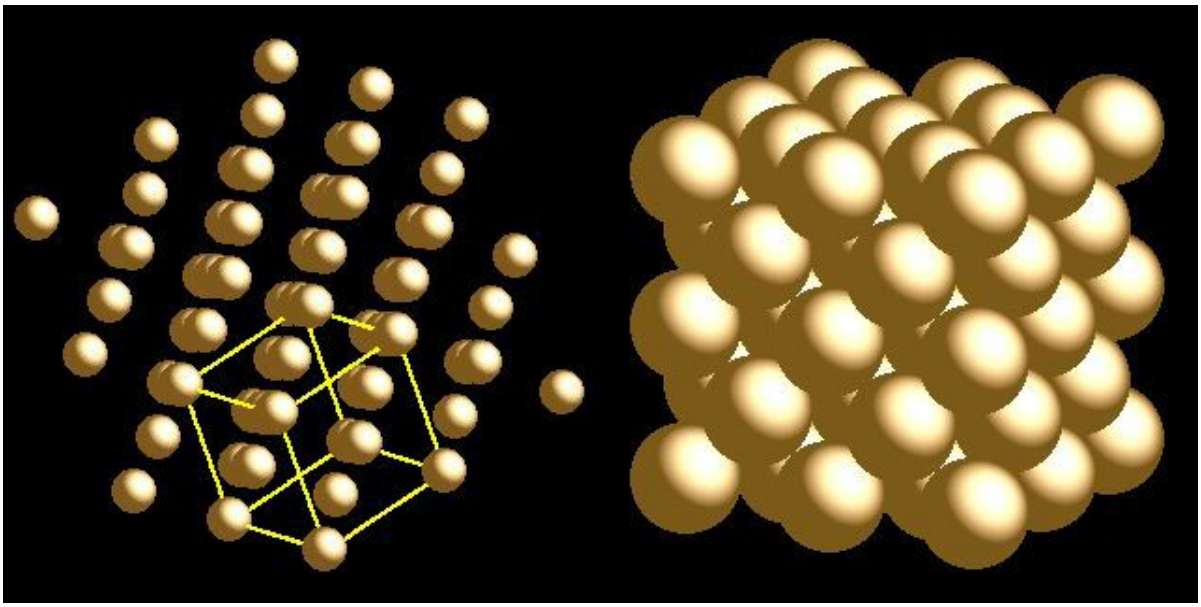
Fig. 1 XRD patterns of an amorphous ITO gel after evaporation of the solvent, ITO powder after calcination at 400 °C and an ITO thin film. The gel and the powder were prepared with acetic acid and ethylene glycol, an initial cation concentration of 0.125 M and 5 cation% Sn. The film with 10 cation% Sn was prepared by 10 subsequent depositions. The pattern for the powder and the film could be indexed to the cubic In2O3 with the space group Ia[3 with combining macron] given at the bottom. The broad bump at around 25° in the diffractogram of the ITO thin film is due to the amorphous glass substrate.

Gold

Crystal structures

- Space group: **Fm-3m**
- Space group number: **225**
- Structure: **ccp (cubic close-packed)**
- Cell parameters:

  a: 407.82 pm
  b: 407.82 pm
  c: 407.82 pm
  α: 90.000°
  β: 90.000°
  γ: 90.000°



The closest Au-Au separation is 288.4 pm implying a gold metallic radius of 144.2 pm

References

A. Maeland and T. B. Flanagan, *Can. J. Phys.*, 1964, **42**, 2364.

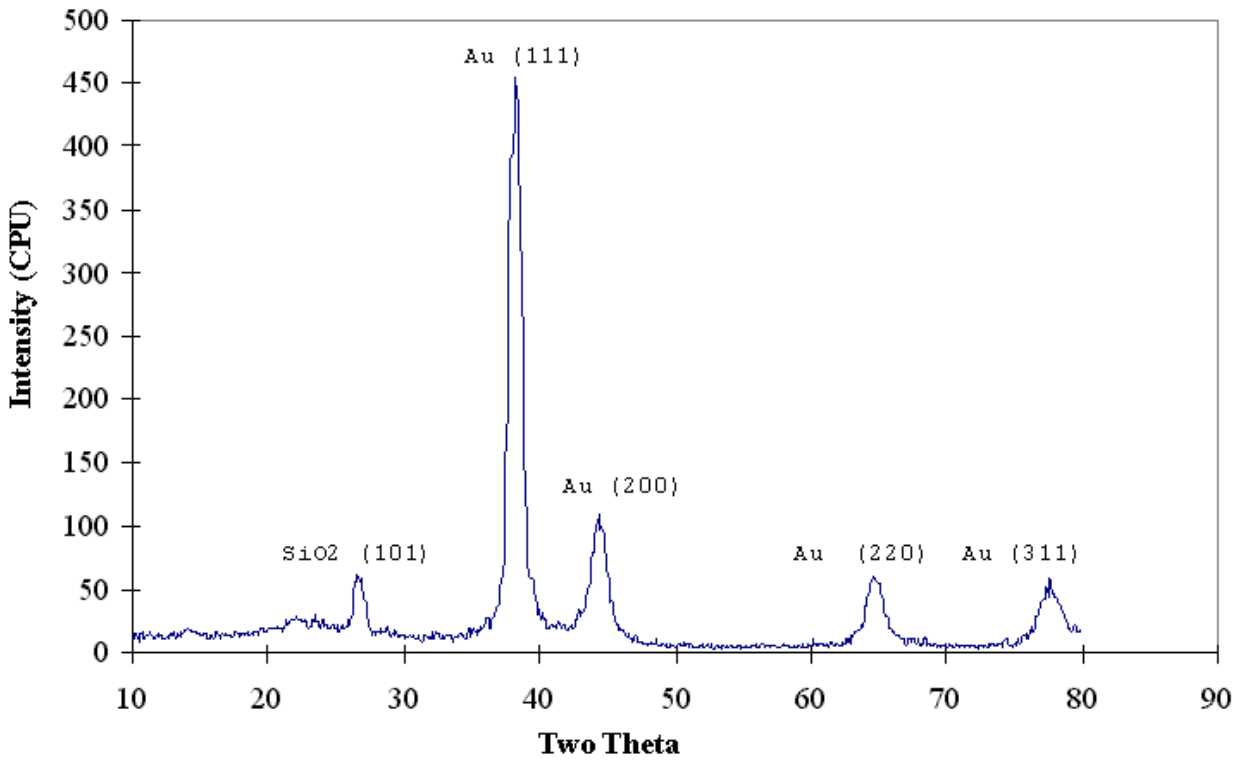
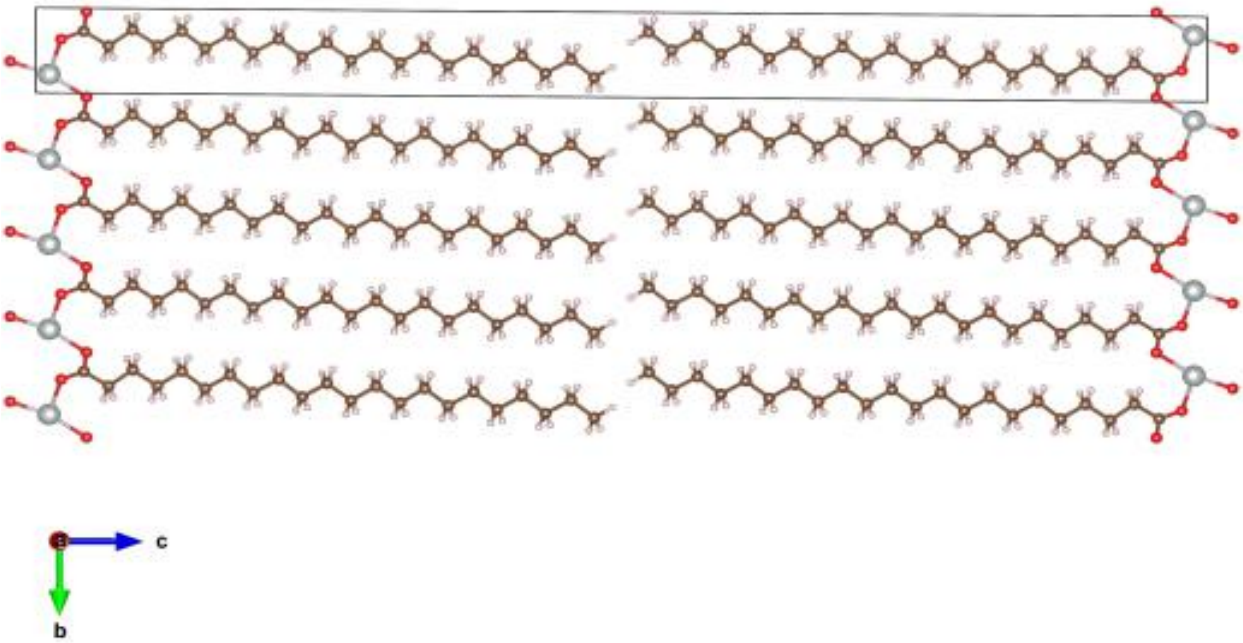


Figure 2. X-ray diffraction pattern of gold electrode coating on a quartz substrate.

Silver behenate

Silver behenate, a crystalline long-chain silver carboxylate, CH3(CH2)20COOAg, has been shown to be a useful material for low- angle calibration of X-ray diffraction instruments (Huang et al., 1993; Blanton et al., 1995a,b). The (0 0 l) long-period spacing of 58.38 Å is a result of a tail-to-tail alignment of two silver behenate molecules in a unit cell (Blanton & Whitcomb, 1999).

What does it look like?



Carbon atoms are brown, oxygen red, hydrogen pink and silver are, well, silver atoms here! Image generated by the VESTA (Visualisation for Electronic and STructural analysis) software http://jp-minerals.org/vesta/en/

What is it?

This is one of the materials behind thermal printing. It's a dry material that when exposed to heat leaves behind silver nanoparticles that are capable of absorbing enough light to be viewed. It also has a really interesting diffraction pattern, with strong peaks at low angles from the large spacing between the silver atoms.

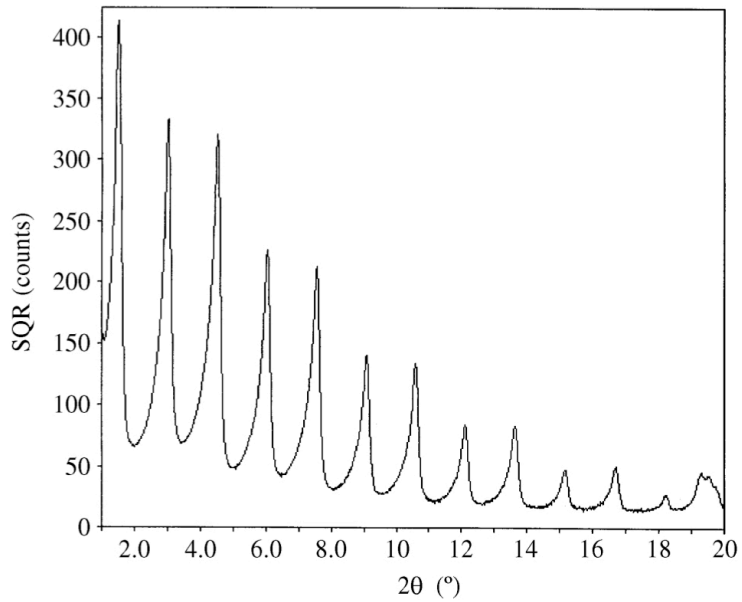
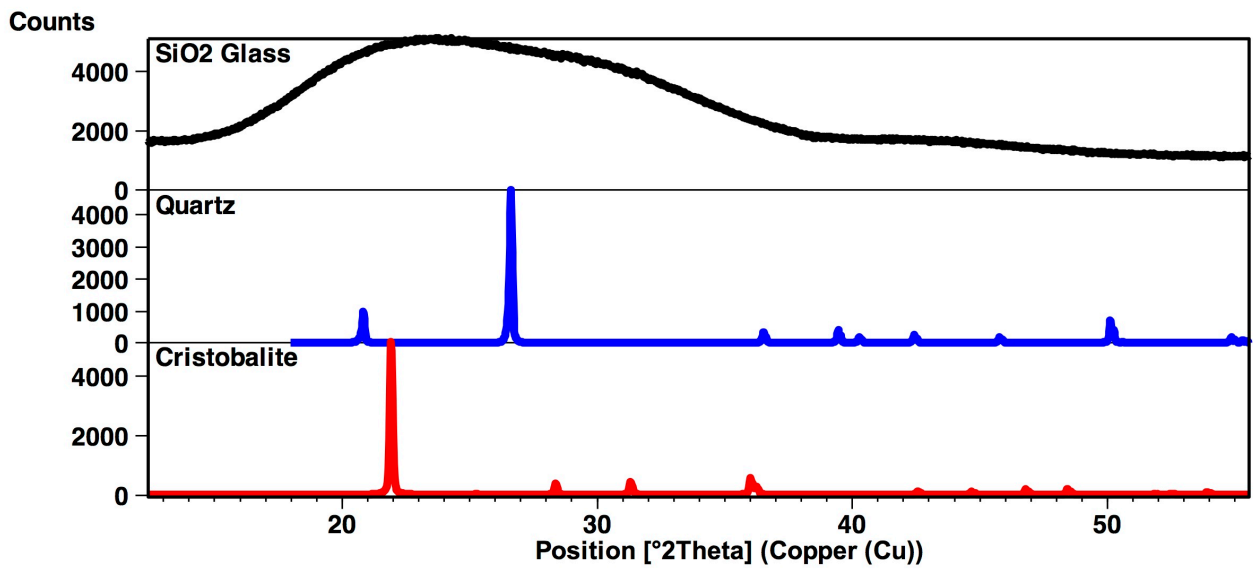


Figure 1
X-ray diffraction pattern of silver behenate powder, front packed into the sample holder, recorded using a laboratory Bragg–Brentano diffractometer (Cu *Kα* radiation).

A typical diffraction pattern of a film of silver behenate. This means it's been really useful as a standard for people doing small-angle diffraction.

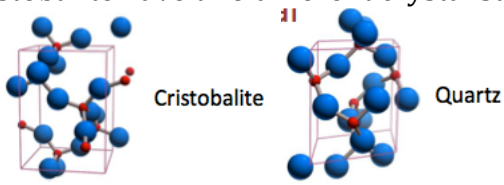
Where did the structure come from?
The crystal structure of silver behenate was determined from powder diffraction in 2011 by Blanton *et al.*, and you can find it in the Crystallography Open Database, #1507774.

Glass



The three X-ray scattering patterns above were produced by three chemically identical forms of SiO2

- Crystalline materials like quartz and cristobalite produce X-ray diffraction patterns
  - Quartz and cristobalite have two different crystal structures



  - The Si and O atoms are arranged differently, but both have long-range atomic order
  - The difference in their crystal structure is reflected in their different diffraction patterns
- The amorphous glass does not have long-range atomic order and therefore produces only broad scattering features