Atomic resolution neutron holography

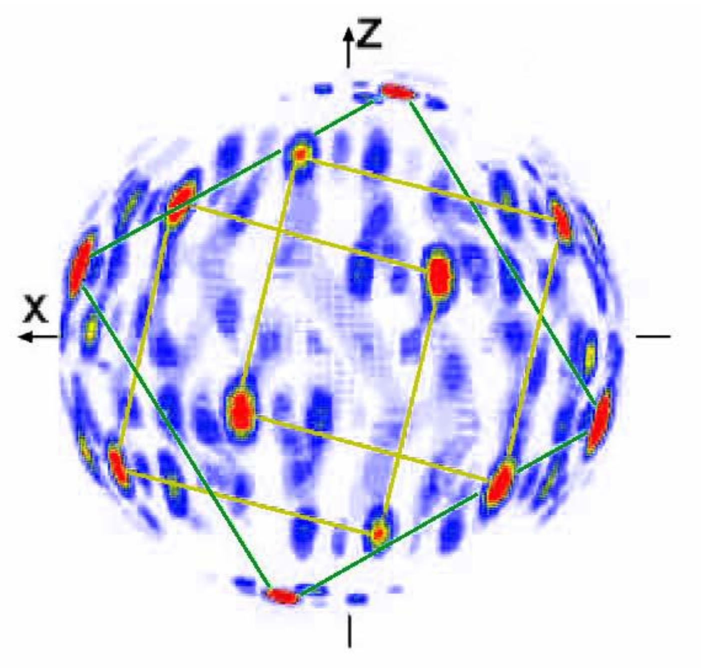
Optical holography uses light waves, normally generated by a laser, to produce three dimensional images of objects. From a physical point of view, it is the interference and diffraction of waves that is the key to process. In principle, a hologram can be produced with any sort of radiation, with the aid of some computation to translate the results into a wavelength that the human eye can see.

Holography with electrons (Szöke, 1986) and X-rays (Tegze and Gaigel, 1996) achieved atomic resolution, that is, they were able to produce images at the atomic scale, where individual atoms are observed. The drawback of using electrons is that they stay at the surface and cannot probe the bulk of a material. X-rays can penetrate much deeper, but their sensitivity varies orders of magnitude along the periodic table, and they are strongly absorbed by heavy elements, which limits their application in many cases.

Thermal neutrons do not have these drawbacks, but a series of challenges must be solved to make it work in practice. This is what Dr. Bhaskar Sur from the Chalk River Laboratories of the Atomic Energy of Canada Limited and Dr. László Cser from the Wigner Research Centre for Physics in Budapest, Hungary, and their co-workers, did, almost at the same time (Cser et al, 2001, Sur et al., 2001).

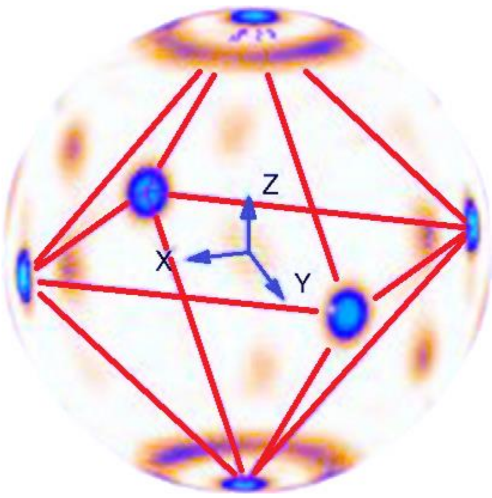
Some of the challenges were technical, such as improvements in the detection systems. Other difficulties arise from physical principles: the neutrons can interact with matter in a number of ways, and some of those ways, such as elastic diffuse scattering, lead to a strong non-holographic signal that can mask the hologram. Distortions and parasitic signals are also inherent to the method. Cser and co-workers developed a new reconstruction method that minimizes the distortions (Markó et al., 2010).

The figure shows the positions of 12 lead atoms surrounding a cadmium nucleus (Cser et al., 2006), in a diluted Pb(Cd) system where there is one cadmium atom for each 380 lead atoms.



Lead atoms around a Cd atom. Adapted from L. Cser et al., Physica B 385–386 (2006) 1197.

The crystal lattice around the cadmium could be determined from the hologram, and the distances between individual atoms could be determined with extremely high precision, 0.01 Å which is less than 1% percent of the interatomic distance. In the figure, only the first shell of lead neighbors around the cadmium is shown, but four neighboring shells could be observed. This enables studies of local distortions of the atomic structure on an unprecedented local scale. A similar example is shown below where palladium atoms around a hydrogen atom are visualized.



Palladium atoms around a hydrogen atom in a $PdH_{0.78}$ structure. Adapted from L. Cser et al., Physica B 385–386 (2006) 1197.

Other applications can use the magnetic properties of the neutrons to study the local magnetic structure around a specific nucleus embedded in a crystal lattice (Szakal et al., 2015). In any case, atomic resolution neutron holography of polycrystalline structures is a very recent development that opens up new fields of application (Szakal et al., 2015), such as resolving the 3D structure of membrane protein structures so far inaccessible to any other technique.

How does neutron holography work?

Optical holography is used to produce a three dimensional image of the subject. A light beam, usually produced by a laser, is split in two equal beams. One of them illuminates directly the object, where it scatters towards the recording medium. The second (reference) beam incises directly on the recording medium. The two beams produce an interference pattern, which contains the information about the object's image. The recording medium itself does not contain any image. The three dimensional image is reproduced when a light beam, equal to the original, illuminates the hologram. It is diffracted by the interference pattern recorded, producing the actual 3D image observed.

The principle of neutron holography is the same but the practical realization is quite different. There are two different methods. The first method uses the point-like inside-source concept. Thermal neutrons incise on the object, which must contain nuclei that scatter neutrons incoherently, i.e. in all directions. Hydrogen is the best candidate nucleus for this method, because it has an extremely high probability for incoherent scattering. The scattered neutron forms a spherical wave, propagating in all directions. The part of the wave that incises on neighboring nuclei has the role of the illuminating beam. The part of the wave that goes directly to the detector without being scattered off any nucleus has the role of reference beam. The detector records the interference pattern of the two beams, i.e., the hologram.

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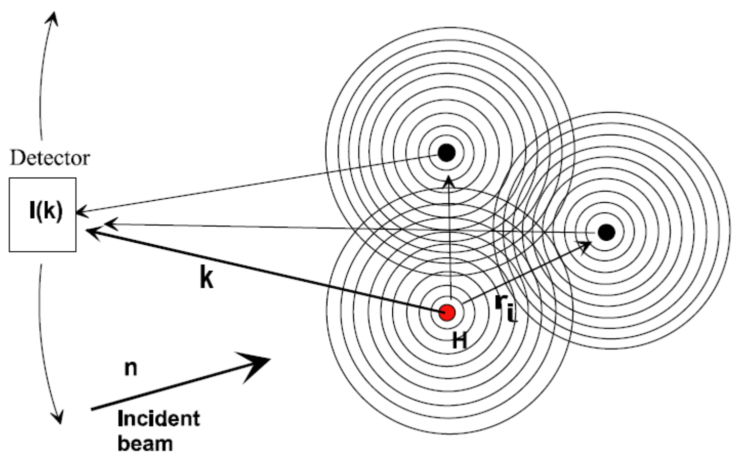

Fig. 1. A monochromatic incident neutron beam illuminates the sample. Neutrons *incoherently* scattered by hydrogen nuclei form spherical waves. The detector which is placed at a larger distance can be reached by these waves either directly or after having undergone a *coherent* scattering process by neighboring nuclei. By moving the detector along the surface of a sphere around the sample the interference pattern of these waves can be recorded.

The second method uses the point-like inside detection concept. A neutron beam generated far enough that it can be considered to be a plane wave incising on the sample, which must contain nuclei with a strong neutron capture reaction that emits gamma radiation has a product. Cadmium is one such nuclei. The direct beam that reaches the cadmium functions as the reference beam. Neutrons that are coherently scattered off neighboring nuclei have the role of illuminating beam. The gamma emission is modulated by the resulting neutron density at the cadmium nucleus. The sample is rotated while the gamma rays are detected, thus acquiring the interference pattern that forms the hologram.

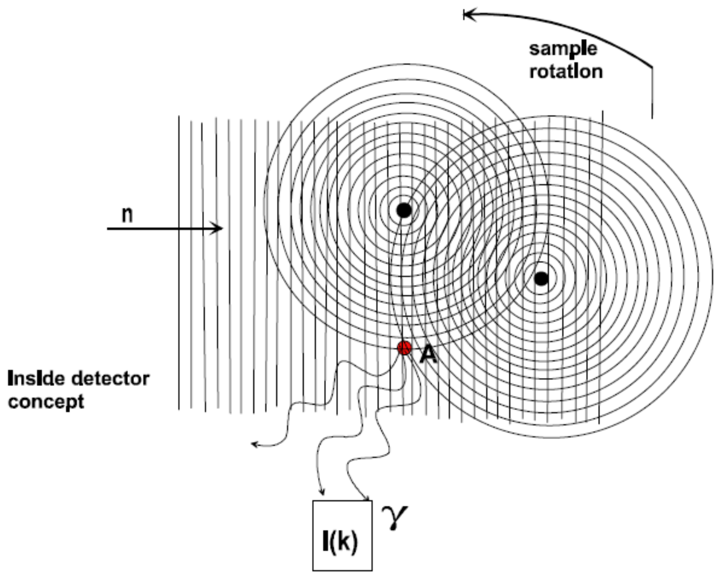

Fig. 2. A monochromatic plane neutron wave emitted by a distant source propagates towards the target nucleus and at the same time serves as the reference beam. The scattered part of the wave forms the object beam and interferes with the reference wave. The resulting neutron density modulation is converted by the detector nucleus (more precisely: many detector nuclei) into intensity modulations of the prompt γ-rays. The intensity $I(\boldsymbol{k})$ of these γ-rays is registered by the detector.

In both experimental methods, the hologram is simply a set of neutron or gamma yields as a function of detector or sample position. The images are obtained as a result of involved calculations that take into account the physical processes of neutron scattering.

Pictures credit: (Cser et al., 2004) .