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Citation: The Physics Teacher **46**, 109 (2008); doi: 10.1119/1.2834534
View online: http://dx.doi.org/10.1119/1.2834534
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Optical Simulation of Debye-Scherrer Crystal Diffraction

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In this paper we describe and discuss simple, inexpensive optical experiments used to simulate x-ray and electron diffraction according to the Debye-Scherrer theory. The experiment can be used to address, at the high school level, important subjects related to fundamental quantum and solid-state physics.

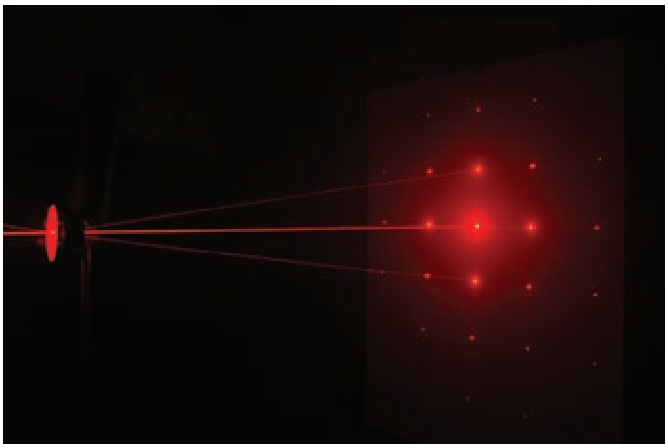

Fig. 1. Low-power red laser (HeNe, 15 mW, λ = 0.6328 μm) diffracted by a two-dimensional grating.

X-ray diffraction is a powerful tool in the analysis of several properties of crystals, as well as of other organic and inorganic substances. W.H. Bragg and W.L. Bragg were able to introduce a simple model in terms of which crystals, such as NaCl and KCl, were understood through their interaction with x-rays. According to this approach, x-rays are reflected by different planes constituted by the points defining the crystalline lattice. Constructive interference of reflected rays occurs when $n\lambda = 2d \sin \theta$ (Bragg law), in which λ is the wavelength of x-rays, d is the distance between crystal planes, and θ is the angle between the incident x-rays and the crystal planes. In an actual experiment, the groups of planes leading to interference maxima are found by letting the crystal rotate slowly. In the so-called x-ray powder diffraction method, referred to as the Debye-Scherrer technique, the sample is first pulverized. The enormous number of crystalline grains leads to independent, randomly distributed constructive Bragg conditions. So, the diffracted beams form cones whose intersections with the detection screen are rings having different diameters. This technique is widely used to identify unknown crystals since characteristic diffraction peaks are produced by each fragment. Information is also obtained about crystal orientation and lattice parameters. X-ray crystallography also allows verification of the de Broglie hypothesis concerning the wave behavior of matter particles. These ideas are currently used in lecture demonstrations to support the wave nature of electrons.[1] In such demonstrations, electrons are diffracted due to their interaction with a very thin polycrystal composed of randomly oriented crystalline regions. This leads to a diffraction pattern similar to that obtained in the Debye-Scherrer setup since the microscopic parts of the polycrystal produce independent, statistically distributed interference patterns.

Our Experiment

For the purpose of introducing at the high school level some of the above-mentioned ideas in modern

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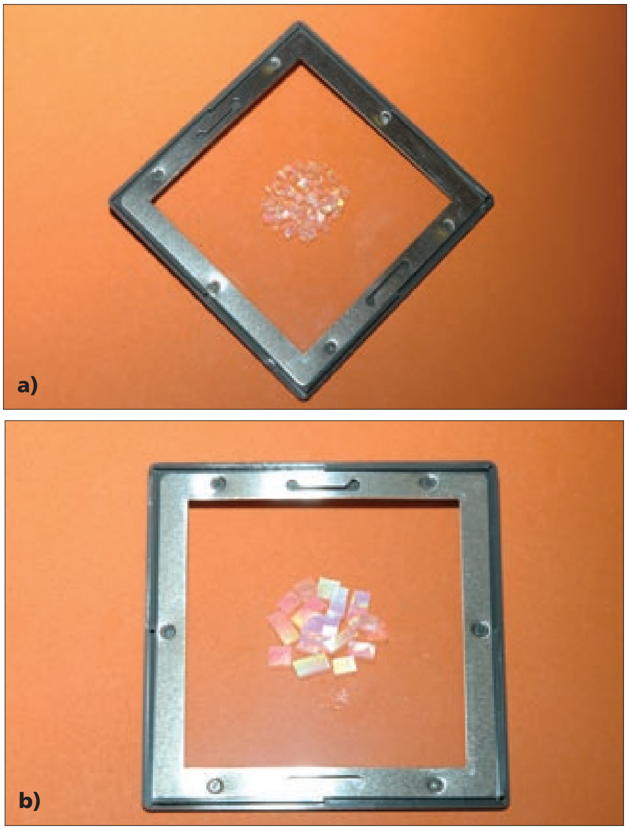

Fig. 2. (a) The grating is cut into small fragments and placed, with random orientation, in a slide frame. (b) A "coarse" version of the fragmented grating in Fig. 2(a); a smaller number of fragments has been used. These have larger dimensions and cover the same area of the previous experiment.

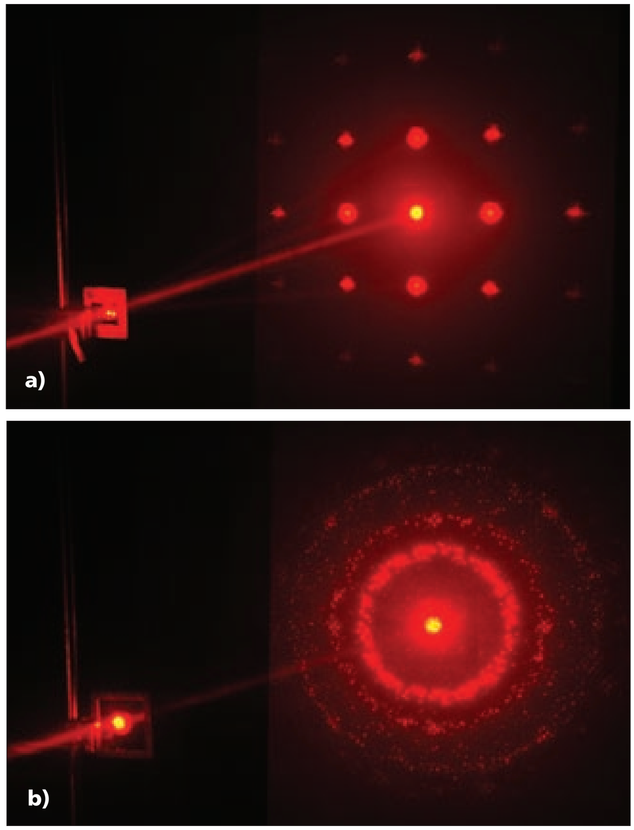

Fig. 3. The laser beam of Fig. 1 is diffracted (a) by the uncut grating and (b) from the fragments shown in Fig. 2(a). Rings due to a Debye-Scherrer condition are clearly visible in the photograph. When the figures are superimposed, the diffraction spots fall on the Debye-Scherrer rings.

physics (which also have a huge number of technical and practical applications), we present in this paper some simple and inexpensive optical experiments analogous to the Debye-Scherrer and Laue diffraction of x-rays and electrons.[2]

As a first step, we consider the diffraction pattern obtained with a two-dimensional optical grating.[3] Such a device can be seen as a series of regularly spaced scattering centers, just as in the case of atoms in a plane within a perfect crystal. Thus, an incident laser beam will be diffracted in a way that depends on the lattice geometry and the wavelength of the light[4] (see Fig. 1).

For our second step, we cut this same (plastic) grating into small pieces (for instance, squares measuring about 2 mm on a side). These pieces are then distributed randomly and framed as shown in Fig. 2. The incident laser beam is expanded by means of a lens so that it can intercept a large number of the grating fragments.

One then observes diffraction rings similar to those obtained in x-ray and electron diffraction experiments since the grating pieces provide a fair simulation of the randomly distributed structure of polycrystals in a powder sample (see Fig. 3).

It is important for students to notice that if a two-dimensional (intact) grating is rotated while illuminated by the laser beam, the diffracted light beams also rotate, tracing out circles on the observing screen. The rings superimpose perfectly on those obtained with the cut-up grating (Fig. 4).

The diffraction rings are defined by several bright spots, each of which is due to the diffraction from a single piece of the grating. This can also be shown by using a sample that has a smaller number of grating pieces (see Fig. 5). The contributions to the overall

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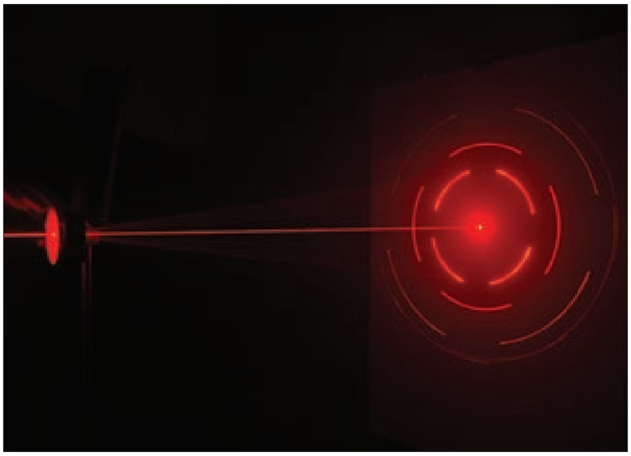

Fig. 4. The grating of Fig. 1 is slowly rotated by hand about the laser beam while the camera shutter is left open. The rotation of diffraction spots leads to rings corresponding to those obtained with the cut-up grating.

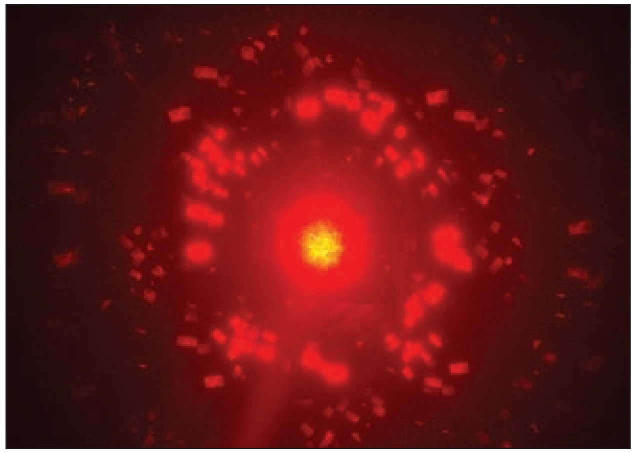

Fig. 5. Diffraction pattern obtained with the cut-up grating shown in Fig 2(b). Single diffraction spots are clearly visible.

diffraction pattern from single pieces of the grating may be seen—the rings are now clearly made up of discrete spots rather than continuous lines. This is because the small number of grating fragments can have only a relatively small number of different orientations.

Real polycrystals behave quite similarly. Actual crystallites in a polycrystalline sample can have quite large dimensions (100 Å - 500 Å).[5] If the sample used in the x-ray powder diffraction experiment contains relatively large grains, the diffraction rings can appear somewhat speckled. In order to obtain more uniform diffraction rings in an actual Debye-Scherrer measurement, the sample is rotated as the photographic exposure is made.

In Fig. 6 we show results of similar experiments using a low-power green laser (5 mW, $\lambda = 0.532\ \mu$m). Note that the diffraction spots are closer together (and the associated rings have smaller radii) than those obtained using red light.

Conclusions

The experiments described in this paper can be used to verify the theory of light diffraction by a grating. In the Laue diffraction pattern, the bright spots surrounding the central maximum are located approximately on a square lattice.[6] It is possible to show that in the associated Debye-Scherrer diffraction scheme, the ratio of the radii of the first two rings is very close to $\sqrt{2}$ (see also Fig. 7). Moreover, it is possible to determine the lattice spacing from the radius of the first diffraction ring and the distance between the grating sample and the screen. We write $n\lambda = d \sin \theta$, where d is the grating spacing, and θ is the angle between the central beam and one of the rays forming the first ring (see Fig. 7).[5] Calling the radius of the first diffraction ring R and the distance between the screen and the grating L, we can use the small angle approximation to write $\sin \theta \cong R/L$ so that the above equation becomes $d \cong \lambda L/R$.

In the case of our green laser, we had $R = 0.28$ m and $L = 1.0$ m. Using these numbers we calculate $d \cong 1.9\ \mu$m, which corresponds to a grating with a spacing of $\cong 5.3 \times 10^2$ lines/mm, very close to the value claimed for this grating (13,500 lines/in $\cong$ 532 lines/mm). We suggest carrying out even more complex experiments in which several different gratings are superimposed in order to simulate crystal structures that are different from the simple cubic arrangement considered here. After a number of such complex layouts have been studied, an "unknown" lattice structure could be identified from a pattern database as is done in actual x-ray diffraction experiments.

References

1. Leybold (http://www.leybold-didactic.de/data_e/index.html) provides a diffraction tube for electrons in which the adopted polycrystal is a graphite layer (thickness $\cong$10 nm). A similar system is available from Tel-Atomic

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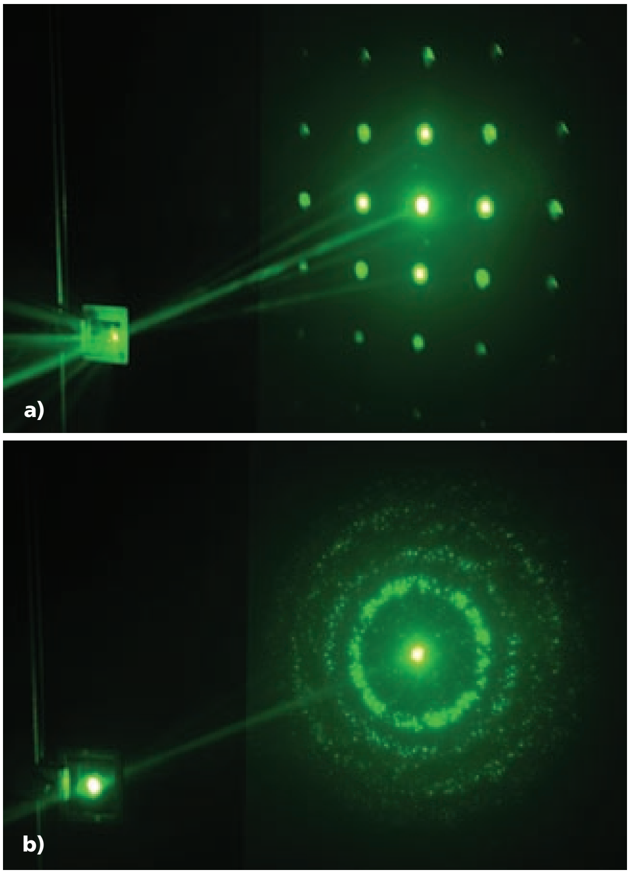

Fig. 6. Diffraction by a two-dimensional grating [intact (a), fragmented (b)] of a green laser beam. These pictures should be compared with Fig. 3. A direct, quantitative comparison is possible since the camera was maintained at the same position and with the same focal length while taking the photographs.

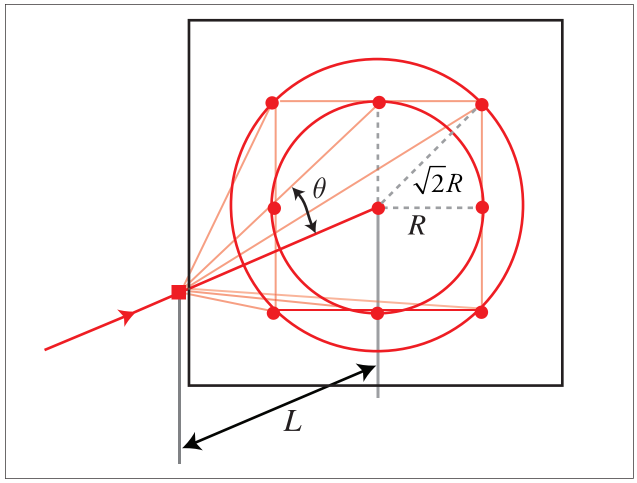

Fig. 7. Schematic respresentation of the x-ray diffraction geometry in a perfect two-dimensional crystal.

(http://www.telatomic.com).

2. Simple experiments in optics about Laue diffraction can be found, for example in Se-yuen Mak, "Gratings for simulation of Laue crystal diffraction," *Phys. Teach.* **32**, 539–541 (Dec. 1994).
3. Two-dimensional gratings are used to make "rainbow glasses." We use holographic 2-D diffraction gratings (Rainbow Symphony, Inc.; http://www.rainbowsymphony.com).
4. Photographs taken with a reflex digital camera (Nikon D70).
5. For a simple, yet detailed introduction to the theory of crystal and polycrystal x-ray and electron diffraction, see, for example, E. H. Wichmann, *Quantum Physics, Berkeley Physics Course,* Vol. 4 (McGraw Hill, New York, 1970), and references therein.
6. A more detailed and thorough treatment of the geometry of diffracted rays by a two-dimensional grating would lead to the result that bright spots do not lie exactly on a rectilinear grid. Actually, they fall on branches of hyperbolae given by the intersections of the Laue cones with the detection screen; see, for example, Ref. 5.

PACS codes: 01.50.Pa, 42.00.00

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