MODELLING TRANSITIONS BETWEEN ORDER AND DISORDER IN A REMOTELY CONTROLLED LABORATORY (RCL)

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1 Introduction

Treatment of wave optics in secondary school physics takes place with special emphasis of description and explanation of diffraction on slits, double slits and grids. Typically, determination of wavelength of the light source (laser), of position of minima and maxima of the diffraction pattern and of the grating parameters are in the focus of the lessons. Only sometimes, the topic is finished by the discussion of the intensity distribution utilizing Feynman's vector formalism in a qualitative manner. Later on, wave optics comes back into the lessons when dealing with solid state physics or the more related crystallography, in particular, when dealing with Bragg diffraction and determination of lattice constants.

In the following, we present an experiment which, on one hand, allows students a qualitative approach to modern crystallography beyond the standard topics like determination of lattice constants in ideal cases and so on. For this purpose we replace the 3D x-ray diffraction technique by an optical analogue, that is diffraction of laser light (by using a cheap laser diode) on 2D models (representing the atoms or molecules of a real solid state lattice). Instead of x-ray scattering at the electron cloud of real atoms or molecules, in the model the scattering of light at motifs of varying shape and arrangement is applied. On the other hand, this experiment can be used to demonstrate and discuss order-disorder transitions on a microscopic level. The first perspective – going beyond standard topics – has several advantages if treated in school:

- It gives an opportunity to introduce crystallography without scare of hazardous experiments, since visible light of relatively low power is used in the model ("optical crystallography"). In particular, as an RCL there is absolutely no risk.
- By comparing the diffraction pattern and the structure of the diffraction objects the students are required to make qualitative - or quantitative (depending on the level) - statements about the causal relations.
- The reduction from 3D crystallography using x-rays to 2D "optical crystallography" using light avoids complications due to absorption, multiple scattering etc.
- Students' concepts about scattering and diffraction will be proven and can be deepened in a more flexible way.
- Going from 1D diffraction objects (*e.g.* slits) – as they are typically applied in school physics – to 2D objects contributes to consecutive knowledge preparing for physics study, but without demanding the pupils.

The second perspective – order-disorder transitions – can be pretty nice modelled by this experimental design of "optical crystallography". Examples from everyday-life are:

- melting of ice (transition from crystal to liquid, increase in entropy),
- heating a solid (increase of displacement due to increase of thermal energy of the constituents),

- liquid crystal displays (disorder-order transition by applying an electrical field),
- change of magnetic properties above Curie temperature (*e.g.* transition from ferromagnetic to paramagnetic state).

Students in secondary school (age ~ 16-18) are familiar with those phenomena although they do not know about the physics behind, in particular on a microscopic level. Therefore, the relation to everyday-life may give an opportunity to motivate students for the topic “order-disorder” and the experimental approach of “optical crystallography” if treated in a context based method. Furthermore, we believe this topic to be appropriate for the students to perform a kind of “mini-research” at school level.

Diffraction objects were designed by a computer algebra program, which then have been reproduced as positives and, further on, developed by photo imaging techniques through the press department of our university. The procedure to generate diffraction objects on slides have been previously described by Koppelmann [1].

2 Learning unit on order-disorder transitions

Fig. 1 gives an overview of the steps within the learning unit with respect to the diffraction objects applied experimentally. Basically, one has to start with an introduction to the model and its relationship to crystallography depending on foregoing tasks like discussing the results of wave optics (about 1D objects) as mentioned above. This procedure contains, *e.g.*, the reduction of the 3D problem to a 2D problem. In addition, it should be clearly pointed out that the diffraction pattern obtained from crystals corresponds to that one of a perfect lattice which is modulated by the (varying) motifs.

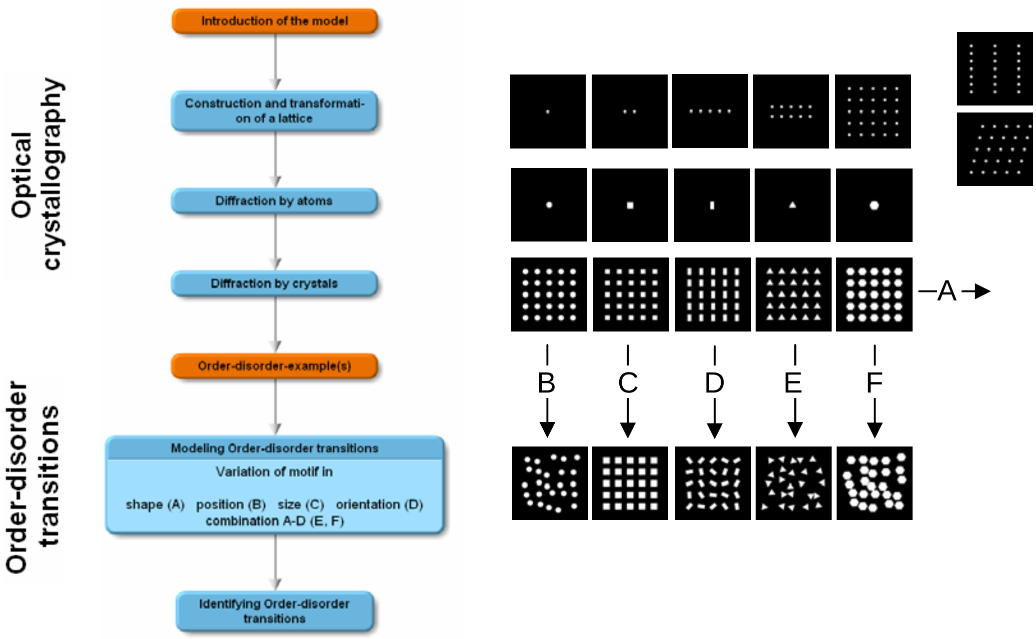


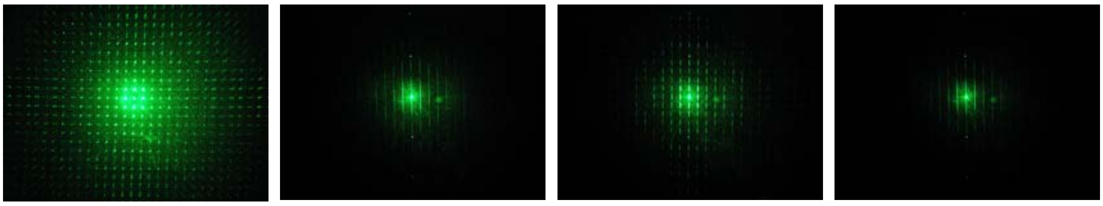
Fig 1. Structure of learning-unit and corresponding application of diffraction objects.

- Learners are required to choose an appropriate model of order-disorder transition on the basis of didactically prepared study guide.
- The changes of the diffraction pattern observed by the learner leads him or her to discuss the structure of the diffraction object.

In the following sections we will briefly discuss several steps, examples and aspects in more detail.

2.1 Construction of a lattice

Fig. 2 depicts the diffraction pattern if going from two holes in a row up to 50x50 holes. By observing the evolution of the pattern when adding holes in *x*- or *y*-direction one can state that the diffraction pattern gains intensity. Going to an infinite number of holes with almost zero diameter we then expect a perfect point diffraction pattern as a limit of an ideal crystal lattice.



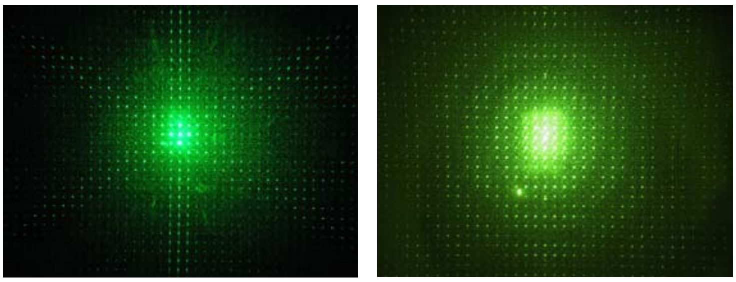
a b c d

Fig 2. Diffraction pattern of 2x1 (a), 50x1 (b), 50x2 (c) and 50x50 (d) holes in a rectangular square lattice, respectively.

In addition, the relation between the point lattice and its reciprocal lattice can be studied by variation of the angle between the 2D lattice vectors.

2.2 Modelling diffraction by real crystals

As can be seen by Fig. 3 the intensity distribution of the ideal lattice is modulated by the diffraction properties of the single object (motif), that is in the case of circular holes (~ rare gas atoms) a radial distribution of intensity, and in the case of a hexagon (~ benzene) a six-fold symmetry of the diffraction pattern. Since we have to deal in real crystals with an enormously large number of atoms or molecules (instead of our diffraction objects for modelling) the peculiar modulation gains intensity. The student's task here is to discuss the impact of the motif of a given atomic/molecular structure on the diffraction pattern, assuming an ideal crystal.



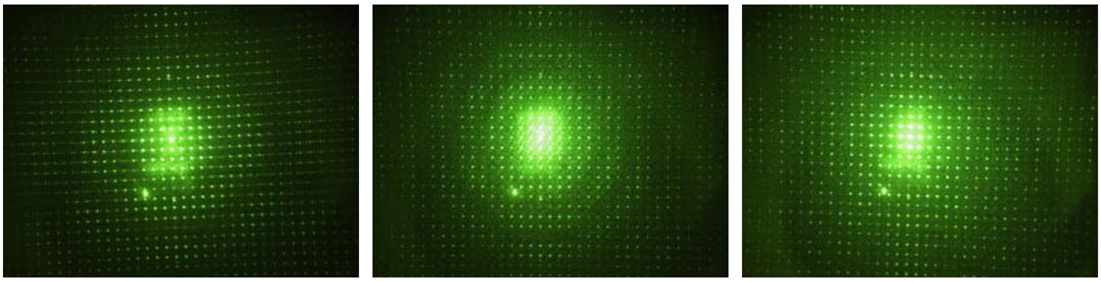
a b

Fig 3. Diffraction pattern of a square lattice with circular holes (a) and hexagons (b).

It can clearly be seen that the more complex a molecule is (*e. g.* circle -> quadratic -> rectangular -> hexagonal) a more complex diffraction will appear. However, the discussion of symmetry properties can be done in school (qualitative) as well as in university (quantitative). At university level, in particular in advanced physics studies, these experiments are useful to make Fourier transformation comprehensible.

2.3 Order-disorder transition: Thermal motion of atoms

Thermal motion of atoms in a crystal lattice is statistical and - in the simplest case - averaged over time it is isotropic. Hence this motion can be modelled by circular diffraction objects with different diameter whereby the amount of thermal motion (~ temperature) corresponds to the diameter of the objects.



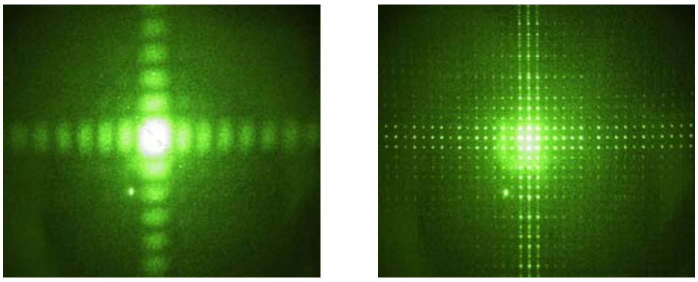
a b c

Fig 4. Diffraction pattern of a square lattice with increasing circle diameter from (a) to (c).

Fig. 4 shows the result of the experiment: the higher the temperature (increasing object diameter) the closer the diffraction rings. In fact, crystal structure analysis has to struggle with thermal motion of the crystal’s constituents, and typically thermal motion of atoms in crystals is represented by so called thermal ellipsoids. Similarly, the size of atoms or spherical molecules (*e.g.* rare gas atoms He -> Ne -> Ar -> Kr -> Xe) can be modelled in this way.

2.4 Order-disorder transition: Solid-Liquid/Gas transition

As an example for solid-vapour transition we modelled a regular 2D lattice containing quadratic motifs by varying statistically the deviation of the “centre of mass” from the ideal lattice points (Fig. 5).



a b

Fig 5. Diffraction pattern of a square lattice build by squares of zero variance (a) and statistical deviation from perfect lattice points (b).

At first sight it is clear that the fine structure representing the regular lattice disappears. Disorder (~ liquid) destroys the coherence, what means that the phase differences of the waves cover a range from 0 to 2π. However, the diffraction pattern due to the “atoms” is still observable since the individual motifs, which are still present, are responsible for it. A simulation of solid-liquid transition, on the other hand, requires the model objects to have a local order remaining, i.e. the next neighbour distance to be similar to the solid case.

3. Realization as a Remotely Controlled Laboratory (RCL)

The concept of an RCL is for a user with a computer from a distant location to remotely control an experiment set up at a specific location (Fig. 6) by means of a web browser. When implementing an RCL one has to take care that the user is able to follow the ongoing real experiment and changes of parameters via web cams as well as gathering the data of the measurements as fast as possible online. Operating the experiment should be as authentic and transparent as possible for the user, *i.e.* the experiment should come across as a common real experiment carried out in lessons or in lab courses.

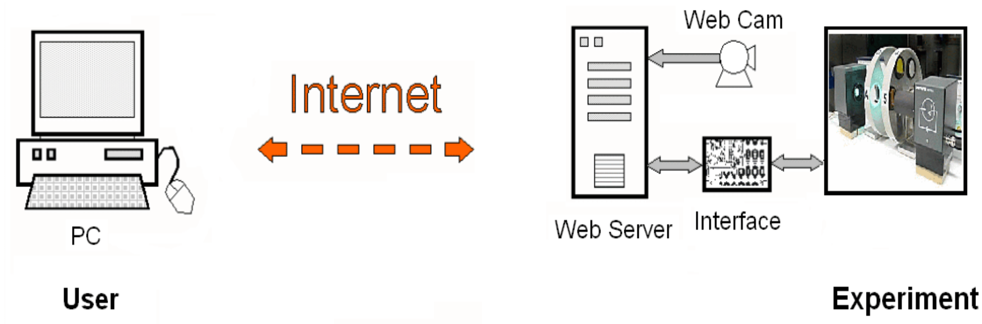


Fig 6. Scheme of an RCL.

Some general advantages of remote controlled labs are: access time 7 days 24 hours, sharing resources between universities and/or schools, opportunity of experimentation which is otherwise not available and flexibility in performing those experiments. In particular, experiments on diffraction and interference in school are limited due to the time available which allows only demonstration experiments, poor variation of parameters and not going into the subject thoroughly including the topics discussed above.

More detailed information about RCLs and the status of the RCL-project can be found in [2]. The RCL "Order-Disorder-Transitions" will be online on our RCL-portal (http://rcl.physik.uni-kl.de) in february 2008.

4. Conclusion

Diffraction and interference is one of the most important topics in secondary school physics, it appears when treating wave optics and solid state physics. However, when treating these topics in school (or in the first semesters of university) standard approaches (*e. g.* 1D cases) are generally applied. A more thorough treatment of diffraction and interference related to everyday context delivers another approach: Modelling of solid state structures, as a first step, and modelling of order-disorder transitions, as a second step, which supports the students' insight in microscopic properties of matter. Moreover, by means of realization of these experiments as an RCL in combination with study guides and learning units students gain the opportunity in explorative learning. Teachers, on the other hand, are provided with material which enables them to teach non-standard topics in the context of everyday-life. Although we could not discuss the learning unit in detail, we think that the presented experiments are convincing. Not only students in school but also students of the first semesters in physics and students in advanced physics studies may benefit the advantages brought by these experiments, in particular, distance learners will benefit from these remote experiments.

5. References

[1] Koppelmann G and Rudolph H 1977 *Photographische Beugungsobjekte für den Unterricht - Herstellung und Eigenschaften* PhuD **3** 220-229

[2] Gröber S, Vetter M, Eckert B and Jodl H-J 2007 *Experimenting from a Distance - remotely controlled laboratory (RCL)* Eur. J. Phys **28** 127-141.