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Experimental simulation research based on two-dimensional lattice reciprocal lattice

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Abstract: In this experiment, two-dimensional crystal structures with different symmetries were simulated using metal microspheres. The effect of simulating the lattice constant change of two-dimensional crystals was achieved by changing the diameter of the metal microspheres. The reciprocal lattice of these two-dimensional structures was measured using a laser as the light source, and the relationship between reciprocal lattice and lattice symmetry, as well as the relationship between reciprocal lattice and lattice constant, was simulated. By measuring the reciprocal lattice, the mathematical relationship between the reciprocal lattice points and the spacing between crystal planes was also verified, and the crystal plane index represented by the reciprocal lattice points was calibrated. In addition, common errors and error results in the experiment were analyzed.

1. Introduction

Crystals are formed by the periodic and regular arrangement of atoms in three-dimensional space, and this three-dimensional periodic distribution can be summarized as lattice translation symmetry. Therefore, this type of lattice is called a crystal lattice (lattice). The reciprocal lattice was established by Ewald in 1921 [1]. It is a virtual lattice obtained from the Fourier transform of a regular lattice, reflecting the symmetry and geometric characteristics of the lattice. The reciprocal lattice is an important concept in physics, which can be used to describe the periodic structure and properties of crystals. However, the concept of reciprocal lattice and its derived reciprocal space differs significantly from actual space, making it difficult to understand.

Based on the above reasons, this article designed this experiment. During the experiment, microspheres were used to simulate the atomic arrangement of a two-dimensional lattice, observe the reciprocal lattice of the two-dimensional lattice, and calculate and calibrate the lattice points of the reciprocal lattice. Firstly, using basic crystallographic knowledge, construct periodic structures with different symmetries and lattice constants; Secondly, by observing and measuring the reciprocal lattice, familiarize oneself with the diffraction knowledge of crystals; Finally, by calculating the reciprocal lattice of different periodic structures, we can grasp the corresponding relationship between lattice and reciprocal lattice, as well as the method of analyzing lattice symmetry and geometric features through reciprocal lattice.

2. Experimental principle of dimensional lattice reciprocal lattice

2.1 Two-dimensional lattice

A crystal is a solid formed by repeating basic units arranged in a certain pattern. Lattices can be divided into different dimensions [2]. A one-dimensional lattice is composed of points on a straight line, a two-dimensional lattice is composed of points on a plane, and a three-dimensional lattice is composed of points in space.

A two-dimensional lattice can be represented by two nonparallel basis vectors a and b, which refer to the smallest vector that can represent the positions of all crystal cells. The position of any crystal cell can be expressed as an integer multiple of the base vector, i.e.

$$R = ma + nb \tag{1}$$

Where n and m are integers. According to symmetry, there are five basic types of Bragg lattices in two-dimensional lattices, namely square, rectangular, rhombic, hexagonal, and oblique, as shown in Fig 1.

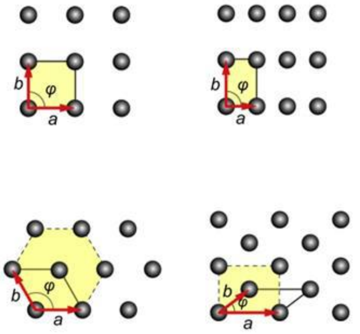


Figure 1: Five types of two-dimensional Bravais lattices

These five types of two-dimensional lattices can be distinguished by two parameters, namely the angle between the basis vectors and the ratio of the basis vectors, as detailed in Table 1.

Table 1: Two dimensional Bravais lattice parameters and reciprocal lattice features

2D lattice type	Reciprocal lattice type	Angle between base vectors	Angle between reciprocal basis vectors	Ratio of base vectors	The ratio of reciprocal basis vectors
square	square	90 °	90 °	1	1
rectangle	rectangle	90 °	90 °	≠1	≠1
diamond	diamond	≠90°	≠90°	1	1
hexagon	hexagon	60 °or120 °	60 °or120 °	1	1
rhombus	rhombus	≠90°	≠90°	≠1	≠1

2.2 Reciprocal lattice

Each lattice point in the reciprocal lattice corresponds to a crystal plane in the actual lattice. The symmetry and spacing of lattice distribution in reciprocal lattice can reflect both the orientation and spacing of crystal planes [3]. For the reciprocal lattice of a two-dimensional lattice, its fundamental vectors can be calculated from the lattice's fundamental vectors:

$$a^* = \frac{b \times n}{|a \times b|} \tag{2}$$

$$b^* = \frac{n \times a}{|a \times b|} \tag{3}$$

The reciprocal space of a two-dimensional lattice can be constructed by translating the basis vectors of the reciprocal lattice:

$$G = ha^* + kb^* \tag{4}$$

Where n and m are integers.

The relationship between the fundamental vectors of a two-dimensional lattice and its reciprocal lattice satisfies the following equation:

$$a \cdot b^* = b \cdot a^* = 0 \tag{5}$$

$$a \cdot a^* = b \cdot b^* = 1 \tag{6}$$

Fig 2 shows the relationship between the lattice basis vectors of a two-dimensional diamond lattice and the basis vectors of its reciprocal lattice.

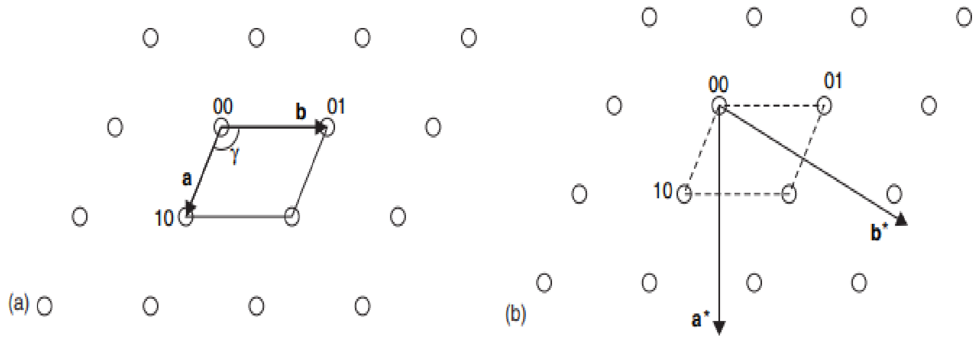


Figure 2: Drawing method of diamond lattice and its reciprocal lattice

2.3 Reciprocal lattice and crystal plane spacing

When light is irradiated on a crystal, diffraction occurs, and the diffraction conditions satisfy the Bragg formula:

$$2d\sin\theta = \lambda \tag{7}$$

The properties of the Bragg formula can be simply and clearly represented by the Ewald diffraction sphere plotting method, as shown in Fig 3. The Ewald sphere plotting method clearly depicts the relationship between incident light, diffracted light, diffracted crystal planes, and reciprocal lattice during the diffraction process [4]. Each point in the reciprocal lattice corresponds to a certain crystal plane in the actual lattice, which can reflect both the orientation of the crystal plane and its crystal plane spacing.

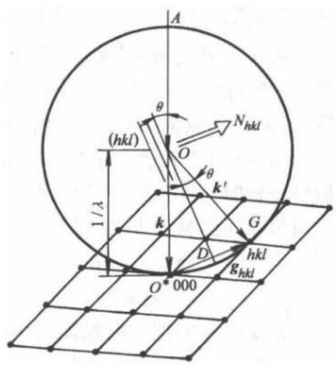


Figure 3: Ewald's sphere drawing method

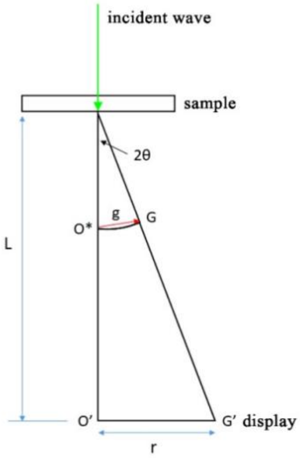


Figure 4: Diffraction geometry of light passing through crystals

Make a sphere with O point as the center and $\frac{1}{\lambda}$ as the radius, and the incident wave vector is $\vec{k}(k=\frac{1}{\lambda})$. The endpoint O^*serves as the origin of the reciprocal lattice. When the reciprocal lattice point G falls exactly on the spherical surface of the Ewald sphere, the crystal plane group represented by the lattice point (with a crystal plane spacing of d) and the direction of the incident light must satisfy the Bragg diffraction formula [5-8]. At this time, the diffraction wave vector beam $\overrightarrow{k'}$ is in the direction of the line connecting the center O of the sphere to the lattice point OG, with the size of the radius $\frac{1}{\lambda}$ of the reflecting sphere. According to the definition of the reciprocal vector:

$$\overrightarrow{k'} - \vec{k} = \vec{g} \tag{8}$$

$$g = \frac{1}{d} \tag{9}$$

Fig 4 shows the geometric relationship of diffraction when light passes through a crystal. Among them, G is the projection grid point of the diffraction light generated by the crystal plane corresponding to the reciprocal lattice G that falls on the Ewald sphere on the computer display, and its distance from the center grid point is r. L is the distance from the sample to the computer monitor, which is related to the optical system used in the experiment and needs to be measured during the experiment.

3. Experimental design ideas and plans

3.1 Design philosophy

Arrange metal microspheres according to the atomic arrangement of a two-dimensional lattice to simulate the atomic arrangement of a two-dimensional lattice. Laser is used to irradiate the lattice arranged in microspheres, which is received by a CCD camera and the reciprocal lattice of the lattice is presented on a computer display. By changing the diameter of metal microspheres, the relationship between lattice and reciprocal lattice is studied. By calculating the distance and angle relationship between reciprocal lattice points, the atomic plane represented by reciprocal lattice points is calibrated.

3.2 Experimental plan

Arrange the metal microspheres on the mobile phone glass film in a two-dimensional lattice atomic arrangement. The glass phone film has good transparency and does not introduce additional interference during optical measurement [9]. Additionally, there is adhesive on one side of the phone film, which can be used to fix metal microspheres. The microspheres do not move during measurement, as shown in Fig 5.

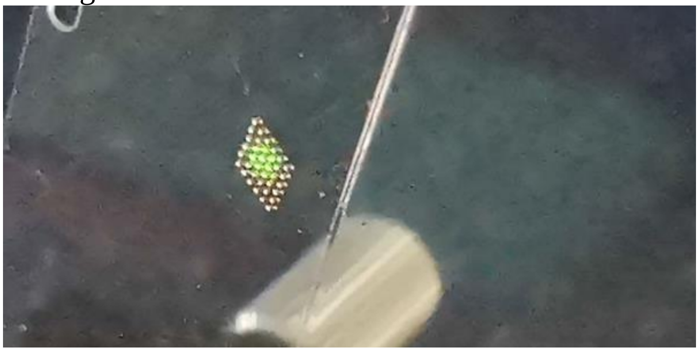


Figure 5: Laser beam vertically irradiated on the sample

4. Construction and measurement process of experimental equipment

4.1 Construction and adjustment of optical testing platform

The distance between reciprocal lattice points and the spacing between lattice planes is related through diffraction. The formula contains unknown parameters that are related to the optical system being constructed. In addition, the reciprocal lattice is usually measured in pixels when presented on computer displays, as shown in Fig 6.

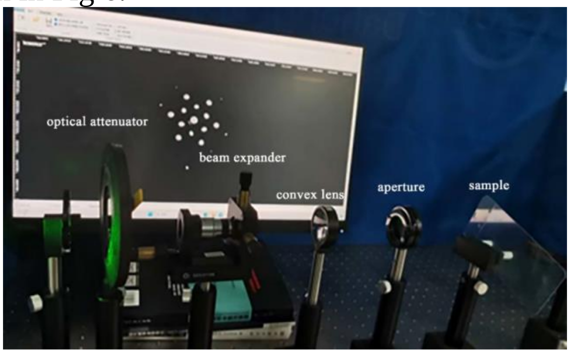


Figure 6: Optical testing platform

4.2 Measurement of constants in optical measurement systems

In order to apply the diffraction formula for further calculations in subsequent experiments, it is necessary to first obtain the numerical value of the constant corresponding to the optical measurement system. In the experiment, multiple known parameters of gratings were measured, and the constants of the optical system were fitted based on the grating measurement results.

Firstly, the diffraction relationship formula $rd = L\lambda$ is transformed to obtain the formula $\frac{1}{L\lambda}d = \frac{1}{r}$.

Based on the formula $\frac{1}{L\lambda}d = \frac{1}{r}$, the value of $\frac{1}{L\lambda}$ was fitted using the least squares method, and finally the $L = 0.0391$ of the optical system used in this experiment was calculated,as shown in Fig 7.

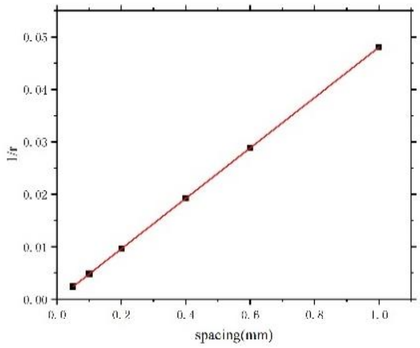


Figure 7: Data fitting diagram of $\frac{1}{L\lambda}$

4.3 Construction of two-dimensional lattice structure

Two types of microspheres with different diameters of 1mm and 0.6mm were used in the experiment[10]. According to the atomic arrangement of the two-dimensional lattice, the microspheres are arranged in an orderly manner on the side of the glass phone film with adhesive, in order to simulate the construction of the two-dimensional crystal lattice, as shown in Fig 8.

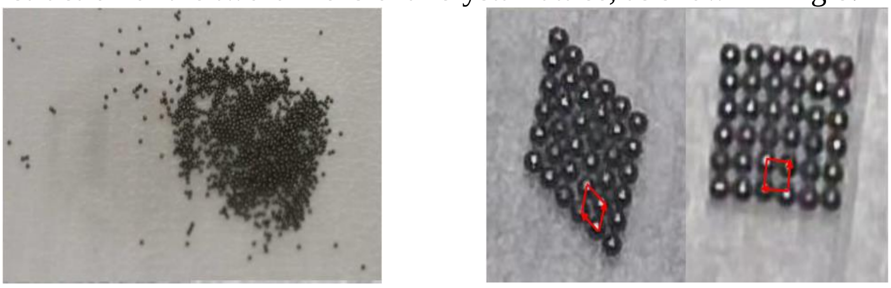


Figure 8: Experimental metal microspheres and ordered arrangement of microspheres to simulate two-dimensional lattice

Figure 9: Measurement diagram of reciprocal lattice

4.4 Analysis of calculation results

The reciprocal dot matrix is presented on a computer screen, and the distance between the dots and the angle between the dots relative to the center half point are measured using pixel measurement tools [11-13]. For convenience, the nearest neighbor (marked in red) and second nearest neighbor (marked in white) of the central grid point ("0") are identified here, as shown in Fig 9.

4.5 The reciprocal lattice of two-dimensional square (hexagonal) lattice

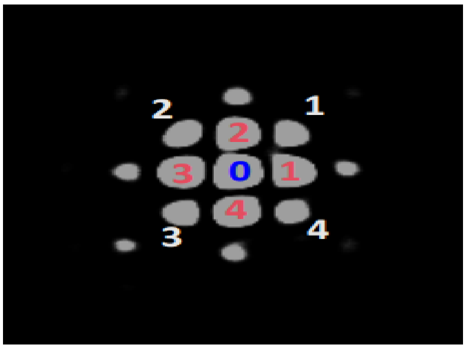
The reciprocal lattice formed by two-dimensional square (hexagonal) lattices simulated with 1mm and 0.6mm diameter metal microspheres under laser irradiation with a wavelength of 532nm was observed and measured through experiments, as shown in Figs 10-13. The measured distance and angle relationships are listed in Table 2-3. It can be seen that the reciprocal lattice of a two-dimensional square (hexagonal) lattice exhibits the same quadruple (sextuple) symmetry as that of a two-dimensional square (hexagonal) lattice, and the distance between the reciprocal lattice points of a 0.6mm microsphere lattice is significantly greater than that of a 1mm microsphere lattice. This reflects the characteristic that the smaller the lattice constant, the larger the distance between the reciprocal lattice points.

Table 2: The distance (in pixels) between the central lattice point and four (six) equivalents nearest neighbor lattice points in a reciprocal lattice

	1mm	0.6mm	(1mm)	(0.6mm)
1	20	34	(24)	(40)
2	20	35	(23)	(39)
3	20	34	(25)	(40)
4	21	35	(24)	(38)

Table 3: The angle between the nearest neighboring lattice point and the central lattice points in reciprocal lattice (unit: degrees)

	1mm	0.6mm	(1mm)	(0.6mm)
∠102	89.8	92.3	(61.7)	(57.8)
∠203	89.5	89.8	(61.3)	(60.5)
∠304	90	91.8	(62.1)	(59.4)
∠401	89.3	90.5	(59.3)	(58.1)
∠506			(61.6)	(60.4)
∠601			(60.7)	(62.3)



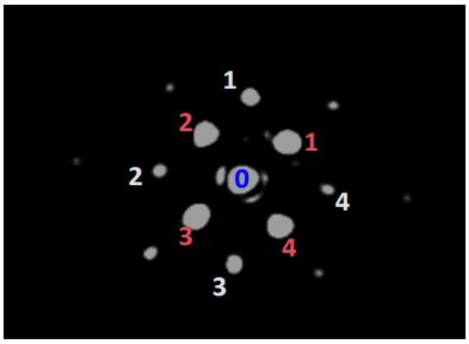
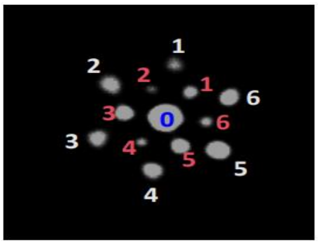


Figure 10: The reciprocal lattice of a square lattice simulated by a 1mm diameter microsphere (Left)

Figure 11: The reciprocal lattice of a square lattice simulated by a 0.6mm diameter microsphere (Right)



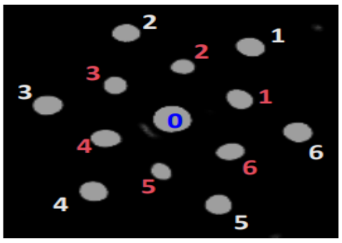


Figure 12: The reciprocal lattice of a hexagonal lattice simulated by a 1mm diameter microsphere (Left)

Figure 13: The reciprocal lattice of a hexagonal lattice simulated by a 0.6mm diameter microsphere (Right)

4.6 Calculation and calibration of two-dimensional square (hexagonal) lattice reciprocal lattice

The symmetry of the reciprocal lattice is consistent with the symmetry of the actual crystal lattice. Each point in the reciprocal lattice corresponds to a crystal plane in the actual crystal lattice. The distance between the reciprocal lattice point and the central lattice point reflects the interplanar spacing corresponding to the crystal plane, and the two are related through Bragg's formula. Through calculation, the crystal planes corresponding to each lattice point of the reciprocal lattice formed by the square lattice and hexagonal lattice constructed of 0.6mm diameter microspheres were calibrated, and the crystal plane spacing was calculated according to the diffraction formula: $rd = L\lambda$ calculate.

In Fig 14-15, the lattice points representing the four (six) crystal planes on the reciprocal lattice are calibrated, and the interplanar spacing of the corresponding crystal planes is calculated. The calculation results are listed in Table 4. The theoretical values in the table are calculated based on geometric relationships.

Table 4: The spacing between the {100} ({10-10}) crystal planes calculated from the reciprocal lattice (unit: mm)

{100}		{10-10}	
-100	0.612	(10-10)	0.52
-10	0.594	(01-10)	0.533
(-100)	0.612	(-1100)	0.52
(0-10)	0.594	(-1010)	0.547
Theoretical value	0.6	(0-110)	0.52
		(1-100)	0.507
		Theoretical value	0.52

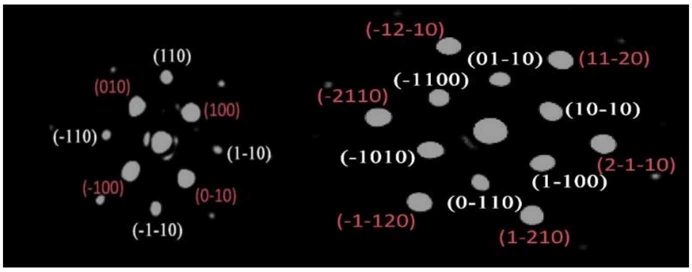


Figure 14: Calibration of the nearest (second) neighbor lattice point of the center lattice of the square lattice reciprocal lattice (Left)

Figure 15: Calibration of the nearest (second) neighbor lattice point of the center lattice of hexagonal lattice reciprocal lattice (Right)

5. Conclusions

This experiment is simple to operate and has high precision, and the experimental supplies such as metal microspheres and mobile phone glass films used to build the two-dimensional crystal structure are cheap and easy to obtain. Innovations were made in experimental research ideas, and the understanding of concepts was deepened by building atomic arrangements and observing the corresponding reciprocal lattice. This experiment is highly scalable. Through different combinations of microspheres, two-dimensional lattice structures with different lattice constants and different symmetries can be built. This experiment well demonstrates the relationship between the crystal lattice and its reciprocal lattice. The lattice has the same symmetry as its reciprocal lattice, and the larger the lattice constant, the smaller the spacing between the reciprocal lattice points. This experimental method is simple and can deepen the understanding of the concept of reciprocal lattice. It has a good teaching effect for those who are familiar with the relationship between reciprocal lattice and crystal symmetry, crystal lattice constant, and crystal plane index.

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