

# Ordered distribution of point defects in alkali-halide crystals

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(Submitted September 6, 1974)

*ZhETF Pis. Red.* 20, No. 8, 551-554 (October 20, 1974)

An ordered distribution of point defects in alkali-halide crystals was observed in experiment. Some of the defects form a lattice, and the others are outside the lattice at certain mean distances from one another.

The character of the distribution of point defects in crystals determines the mechanism and the kinetics of many physical and physical and chemical processes that occur in their volume and on the surface. Therefore the question whether the point defects are disposed at random or in various ordered formations is of great importance for the interpretation of a variety of experimental data and for the development of the theory of such phenomena as processes of luminescence, phase transitions, deformation, diffusion, crystallization, and catalysis. In this article we report observation of an ordered distribution of point defects in alkali-halide crystals.

It was previously established<sup>[1-4]</sup> that nucleation and the relative nuclei on crystal surfaces takes place selectively on point defects. Therefore an analysis of the earlier stages of crystallization (decoration patterns) makes it possible to visualize, on the basis of the distribution of the decorating particles, the microtopography of point defects on the crystal surface, which is a regular reflection of the distribution of the point defects also in the volume of the crystal.

We investigated NaCl single crystals, including  $x$ -irradiated samples. The procedures of decorating with gold and of preparing the samples are described in<sup>[5]</sup>. The distribution of the decorating gold particles was investigated by a small-angle diffraction method after Bassett and Keller<sup>[5]</sup> and by an optical diffraction method<sup>[6,7]</sup> using an instrument described in<sup>[8]</sup>.

A homogeneous diffusion aureole is produced around the nondiffracted electron beam on the pictures of the small-angle electron diffractions from gold particles

separated from the NaCl crystal surface and heated during the decoration time to 250 °C (Fig. 1a). This indicates that the gold particles (and accordingly the point defects) are not disordered, but are spaced with a certain average distance on the order of 180 Å from one another. In addition to this aureole, the picture shows also four elongated rather sharp maxima, which reflect the ordered arrangement of the point defect along the crystallographic directions  $\langle 100 \rangle$  and  $\langle 010 \rangle$  of NaCl, with an average period of 180 Å, i.e., a unique lattice of point defects is produced in the crystals. In this case this lattice is rather strongly distorted, since the elongation of the reflections indicates a scatter of the lattice period. When the NaCl crystals are heated to 300 °C and the decoration is carried out at this temperature, the sharp reflections of the small-angle electron diffraction reflect, as before, the ordered disposition of the point

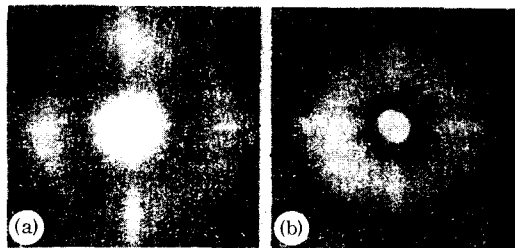


FIG. 1. Patterns of small-angle electron diffraction from decorating gold particles produced on surface point defects of NaCl single crystals. The crystal temperatures were 250 °C (a) and 300 °C (b).

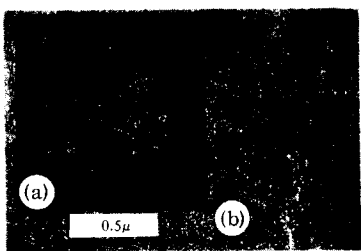


FIG. 2. Optical diffraction (a) from the electron-microscope picture of gold-decorated surface of NaCl sample exposed to x-rays (b).

defects along  $\langle 100 \rangle$  and  $\langle 010 \rangle$  of NaCl. The value of the period in these directions, however, decreases to an average of  $120 \text{ \AA}$  (Fig. 1b). The increase in the sharpness of the reflections indicates a higher degree of perfection of the point-defect lattice. The diffuse aureole breaks up into four smeared-out arcs located at the center of the sharp reflections. It follows therefore that the point defects, which previously were outside the lattice, "become aligned" in the lattice, and this is accompanied both by a change in the periods of the lattice and by a decrease in their scatter.

Irradiation of the NaCl crystals by x-rays leads, like heat treatment, to an increase in the order of the point defects. Optical diffraction from the electron-microscope image of the picture of gold-decoration of an irradiated NaCl sample heated to  $300^\circ \text{C}$  is shown in Fig. 2. The observed reflections correspond to a lattice of point defects, predominantly radiation defects, with a period on the order of  $55 \text{ \AA}$ . The lattice axis, as in

the non-irradiated crystals, are directed  $\langle 100 \rangle$  and  $\langle 010 \rangle$  of NaCl.

The experimental results lead to the important conclusion that point defects in crystals are arranged in two ways: some of the defects form a lattice (or lattices), and the remainder are outside this lattice at certain mean distances from one another. Depending on the heat treatment or on the crystal irradiation (and probably also on other effects), the relative number of point defects inside and outside the lattice can vary significantly.

The ordered arrangement of the point defects (in the limit, the formation of a lattice of point defects with various periods) exists not only in NaCl crystals but also in many crystals investigated by us, and can obviously greatly influence many physical and physico-chemical processes and phenomena that occur in single crystals.

<sup>1</sup>G. I. Distler, *Izv. AN SSSR, Ser. Fiz.* 32, 1044 (1968).

<sup>2</sup>P. W. Palmberg, C. J. Todd, and T. N. Rhodin, *J. Appl. Phys.* 39, 4650 (1968).

<sup>3</sup>G. I. Distler, V. N. Lebedeva, and V. V. Moskvin, *Kristallografiya* 14, 664 (1968) [*Sov. Phys.-Crystallogr.* 14, 559 (1969)].

<sup>4</sup>G. I. Distler, *Izv. An SSSR, Ser. Fiz.* 36, 1846 (1972).

<sup>5</sup>C. A. Bassett and A. Keller, *Phys. Mag.* 2, 817 (1964).

<sup>6</sup>A. Klug and T. E. Berger, *J. Mol. Biol.* 10, 565 (1964).

<sup>7</sup>B. K. Vainshtein and G. I. Kosourov, *Kristallografiya* 11, 921 (1966) [*Sov. Phys.-Crystallogr.* 11, 778 (1967)].

<sup>8</sup>G. I. Kosourov, I. E. Lifshitz, and N. A. Kiselev, *Kristallografiya* 16, 813 (1971) [*Sov. Phys.-Crystallogr.* 16, 702 (1972)].