COMMUNITY OF NATURE BETWEEN WEHNER SPOTS AND THE BLOCKING EFFECT ON PASSAGE OF PARTICLES THROUGH SINGLE CRYSTALS

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A formalism that reveals community of nature between Wehner spots and the blocking effect on passage of particles through single crystals is grounded and developed. The method grew out of the author's work on the theory of the blocking effect, and uses a nonlocal-statistical description of the beam particles, the atoms of the crystal, and the interaction between them.

The following reasons can be advanced for an inquiry into the community of mechanism between the erosion of crystal atoms that results in Wehner spots [1-3] on the one hand and, on the other, the blocking effect of ion motion in the directions of the principal crystallographic axes of a crystal [4-7]. In both cases, there is a center of emission (or scattering) within the crystal. In both cases, repulsive interaction forces between the moving beam particles and the atoms of the crystal are basic.

There is a closed formalism [8-10] of the statistical theory that describes the motion of arbitrary particles in a given periodic crystal field. This formalism is sensitive to details of the interaction of the beam particles with the crystal's atoms.

It is natural to ask whether the qualitative differences between Wehner spots and blocking lunes are merely a result of a quantitative difference in the interaction parameter characterizing the repulsive forces between the atoms of the crystal and the moving beam particles, with preservation of the mechanism translating the particles through the crystal in both cases. If this parameter is determined by the kinetic energy of the particles, there should be a continuous transition of the Wehner-spot pattern to blocking lunes and vice versa as this energy is varied. We shall extend the statistical theory developed earlier for blocking and channeling phenomena to resolution of this problem.

The original statistical theory was based on abandonment of localization of the beam particles and crystal atoms as a primary concept. It was based on continuous particle position, velocity, and acceleration probability fields in the form of the distribution functions

$$\rho(\mathbf{r}, t),\ f(\mathbf{r}, \mathbf{v}, t),\ f(\mathbf{r}, \mathbf{v}, \dot{\mathbf{v}}, t)$$

and the conservation laws for these functions [11-12].

The following problems are posed in this paper.

Develop a statistical apparatus for an arbitrary law of the interaction forces between the moving particles and the crystal atoms in order to unify the mechanisms of motion through the crystal for both ions and neutral particles.

In this interaction law, designate a parameter that is sensitive to changes in the kinetic energy of particle motion. Variation of this parameter would make it possible to verify the basic hypothesis: Do the Wehner-spot and blocking effects merge continuously into one another without any changes in the statistical mechanism of beam-particle translation through the crystal?

The initial equation system for the distribution function of the particles in the beam (f), the crystal-atom position probability (ρ), and the interaction between beam particles and crystal atoms is the same as in [8-10]:

$$\frac{\partial f(\mathbf{r},\mathbf{v},t)}{\partial t}+div_{\mathbf{r}}\,\mathbf{v}f+div_{\mathbf{v}}\langle\dot{\mathbf{v}}\rangle f=$$

$$=\Phi(|\mathbf{v}|)\left(\frac{w_{aa}}{2\pi\theta}\right)^{\frac{3}{2}}e^{\frac{-w_{aa}}{2\theta}r^2},$$

$$\langle\dot{\mathbf{v}}\rangle=\frac{\int\limits_{(\infty)}\dot{\mathbf{v}}f(\mathbf{r},\mathbf{v},\dot{\mathbf{v}},t)\,d\dot{\mathbf{v}}}{f(\mathbf{r},\mathbf{v},t)}=-\frac{1}{m}\,\mathrm{grad}_{\mathbf{r}}\,[U_f(r)+Z_1e\varphi(\mathbf{r},t)],$$

$$U_f(\mathbf{r})=\int K_f(|\mathbf{r}-\mathbf{r}'|)\,\rho(\mathbf{r}',t)\,dr',\quad \Delta\varphi(\mathbf{r},t)=-4\pi Z_1e\int\limits_{(\infty)}f\,d\mathbf{v},\tag{1}$$

$$\rho(\mathbf{r})=C\exp\left[-\frac{U(\mathbf{r})}{\theta}\right],\ U(\mathbf{r})=C\int K(|\mathbf{r}-r'|)e^{-\frac{U(r')}{\theta}}dr'.$$

Here $K_f(|r - r'|)$ and $K(|r - r'|)$ are the potentials of pair interaction between the moving beam particle and atoms of the crystal situated at points r and r' and of the two crystal atoms with one another under equilibrium conditions.

The specific nature of the moving particles is fully determined by the energy $K_f(|r - r'|)$ of the interaction. Therefore, the initial equations are valid for motion of both charged and neutral particles through a given crystalline structure.

The source of particles (charged or neutral) in the crystal is described in the right-hand side of the first equation by the assigned distribution of the beam-particle velocities at the source, $\Phi(|v|)$, and a Gaussian distribution of its position in the neighborhood of the coordinate origin.

Equation system (1) can be used to determine the distributions of the particles moving through the crystal with respect to the assigned source characteristics, the structure of the crystal, and the types of interactions of all particles with one another.

The probability density distribution $\rho(r)$ of the positions of the atoms in the crystal was defined in [8]. For a bounded crystalline plate, it is determined by a Fourier integral series:

$$\rho(\mathbf{r})=\sum_{n_x,n_y=-\infty}^{+\infty}e^{ik_\perp r_\perp}\int\limits_{-\infty}^{\infty}\Big(\sum_{n_z=-\nu_b}^{\nu_a}e^{-in_za_zk_z}\Big)\rho_{\mathbf{k}_\perp k_z}e^{ik_zz}\,dk_z,$$

where

$$\mathbf{k}=\left(\frac{2\pi}{a_x}n_x,\ \frac{2\pi}{a_y}n_y\right),\ n_x,n_y=0,\pm1,\pm2,\ldots$$

$$\rho_{\mathbf{k}_\perp k_z}=\Big(\int\limits_{(\Omega)}\rho\,d\mathbf{r}\Big)\frac{1}{2\pi a_xa_y}\ e^{-\frac{1}{2}\langle x_\alpha^2\rangle(k_\perp^2+k_z^2)},$$

$$\langle x_\alpha^2\rangle=\frac{\theta}{U_{aa}}\Big(\int\limits_{\Omega}\rho\,d\mathbf{r}\Big)^{-1},\ \Omega=a_xa_ya_z.$$

Here a_z is the unit-cell length of the crystal in the direction of the z axis, $\nu_a a_z$ is the thickness of the crystal in the particle exit direction, ν_a is the maximum number of sublattice planes in the crystal through which the particle passes on its way to the collector, and $-\nu_b a_z$ is the distance from the beam particle scattering center to the rear boundary of the crystal.

We shall seek the solution for the particle distribution function in the beam, $f(r, v, t)$, in the form of a series of successive approximations in a parameter that is proportional to the intensity of the atom and atom-ion interactions (i.e., to the charge of the ions in the beam):

$$U_f\to\varepsilon U_f,\ e\varphi\to\varepsilon e\varphi,\ f=f_0+\varepsilon f_1+\varepsilon^2f_2+\ldots,$$

$$\varphi=\varepsilon\varphi_1+\varepsilon^2\varphi_2+\varepsilon^3\varphi_3+\ldots$$

The basis for solution in the form of a series in ε was set forth in [8]. Here we make it our task to obtain the concentration distribution in the beam of particles passing through the crystals without specializing the pair-interaction energy $K_f(|r - r'|)$ in order to establish the sensitivity of the scattering pattern to variations of the beam-particle energy going into $K_f(|r - r'|)$. Following [8], we obtain in the first approximation

$$\int_{(\infty)} \overset{(1)}{f}(\mathbf{r}, \mathbf{v}, t)\, d\mathbf{v} = \rho_f^{(1)}(\mathbf{r}, t),$$

$$\rho_f^{(1)}(\mathbf{r}, t) = -\left(\int_{(\Omega)} \rho\, d\mathbf{r}\right) \frac{1}{m\,|z|^2}\, \frac{a_z}{a_x a_y} \int_{\frac{|r|}{t}}^{\infty} \frac{1}{\xi}\, \Phi(\xi)\, d\xi \sum_{n_z=1}^{\nu_a} n_z \times \tag{2}$$

$$\times \sum_{n_x, n_y=-\infty}^{+\infty} \sigma_f(k_\perp)\, k_\perp^2 \exp\left[-\frac{1}{2}\langle r_\perp^2\rangle k_\perp^2 + i\mathbf{k}_\perp \mathbf{r}_\perp \frac{n_z a_z}{|z|}\right],$$

where

$$\sigma_f(k_\perp) = 4\pi \int K_f(s)\, \frac{\sin k_\perp s}{k_\perp s}\, s^2\, ds,$$

$$\langle r_\perp^2\rangle = \langle x_\alpha^2\rangle + \frac{\theta}{W_{\alpha\alpha}}.$$

We transform (2), using the Poisson summation formula

$$\sum_{n=-\infty}^{+\infty} F(n, x^\alpha) = \sum_{m=-\infty}^{+\infty} \int_{-\infty}^{\infty} F(t, x^\alpha)\, e^{i2\pi m t}\, dt.$$

for the double sum over n_x and n_y.

We then obtain

$$\rho_f^{(1)}(\mathbf{r}, t) = \left(\int_{(\Omega)} \rho\, d\mathbf{r}\right) \frac{1}{m\,|z|^2}\, \frac{a_z}{2\pi} \int_{\frac{|r|}{t}}^{\infty} \frac{1}{\xi}\, \Phi(\xi)\, d\xi \sum_{n_z=1}^{\nu_a} n_z \sum_{m_y, m_x=-\infty}^{+\infty} S(R_\perp). \tag{3}$$

Here $S(R_\perp)$ represents the following dependence of the beam particle density distribution in the plane perpendicular to the symmetry axis:

$$S(R_\perp) = -\int_0^{\infty} k_\perp^2\, \sigma_f(k_\perp)\, e^{-\frac{1}{2}\langle r_\perp^2\rangle k_\perp^2} J_0\left(k_\perp R_\perp \frac{n_z a_z}{|z|}\right) k_\perp\, dk_\perp, \tag{4}$$

$$\left(R_\perp = \left|\mathbf{r}_\perp + (m_x \mathbf{a}_x + m_y \mathbf{a}_y)\frac{|z|}{n_z a_z}\right|\right).$$

We cite the most characteristic of the results obtained.

Formula (3) was derived under the condition that the radius $r_\perp$ of the effective zone of concentration of the beam in the cross-section plane is small compared to the distance $|z|$ to the collector, i.e.,

$$|\mathbf{r}_\perp| \ll \frac{1}{\gamma}|z|, \quad \gamma \gg 1,$$

where γ is an empirical coefficient that describes the properties of the experimental apparatus. The numerical value of this coefficient may determine the largest possible number of Wehner spots or lunes.

We see from the expression for $R_\perp$ that the double sum

$$\sum_{m_x, m_y=-\infty}^{+\infty} S\left(|\mathbf{r}_\perp + (m_x \mathbf{a}_x + m_y \mathbf{a}_y)\frac{|z|}{n_z a_z}|\right)$$

is a periodic function in the x, y plane. The function $S(R_\perp)$ has extreme values at the points

$$\mathbf{r}_\perp = -(m_x \mathbf{a}_x + m_y \mathbf{a}_y)\frac{|z|}{n_z a_z}, \quad m_x, m_y = 0, \pm 1, \pm 2, \ldots$$

When the distance $(d_x, d_y) = (a_x, a_y)\frac{|z|}{n_z a_z}$ between neighboring extremes exceeds the effective width of the function $S(R_\perp)$, the double sum in (3) describes a system of isolated spots that are arranged periodically in the plane of the collector.

The triple sum in (3)

$$\sum_{n_z=1}^{\nu_a} n_z \sum_{m_x, m_y=-\infty}^{+\infty} S(R_\perp) \tag{5}$$

is the result of superposition of spots from different planar sublattices, the total number of which is ν_a. Each of these sublattices produces spots with different periods, widths, and intensities.

The special function $S(R_\perp$ represents the result of intensity distribution in a spot produced by one crystal atom situated in the sublattice numbered n_z and separated from the z axis by the distance $|m_x a_x + m_y a_y|$. The factor $|z|/n_z a_z$ indicates the increase in the scales on projection of the planar sublattices by the beam onto the collector plane.

The special function $S(R_\perp)$ contains information on the basic parameters of beam-particle scattering by the crystal: the force interaction between the beam particles and the crystal atoms, which includes the dependence on the kinetic energy of the beam particles; the lattice constants a_x, a_y, and a_z; the resultant thermal scatter of the atoms around the points of the crystal; and the Gaussian scatter of the center of divergence of the beam:

$$\langle r_\perp^2 \rangle = \frac{\theta}{U_{aa}}\left(\int_{(\Omega)} \rho\, d\mathbf{r}\right)^{-1} + \frac{\theta}{W_{aa}}, \tag{6}$$

where U_{aa} and W_{aa} are the elastic coefficients that characterize the potential wells of the crystal sites and the center of the source.

To include the parameter that depends on the kinetic energy of the moving particles in $K_f(|r - r'|)$, we use the screened potential of the repulsive forces in the Thomas-Fermi model, introducing an impenetrable sphere of radius r_0 into it and assuming

$$K_f(r) = \begin{cases} \dfrac{G}{r}\exp(-\varkappa r), & r \geqslant r_0, \\ \infty & , r < r_0, \end{cases}$$

$$\frac{G}{r_0}\exp(-\varkappa r_0) = \frac{m v_{cr}^2}{2}, \quad |\mathbf{v}| < |\mathbf{v}_{cr}|, \tag{7}$$

where $G = Z_1 Z_2 e^2$ and $\varkappa^{-1} = a_B \cdot 0{,}8853 (Z_1^{2/3} + Z_2^{2/3})^{-\frac{1}{2}}$ for the ions and these parameters are correct in order of magnitude for the atoms; the salient condition requires the existence of an upper limit of the beam particle velocity spectrum (v_{cr}).

It would be more accurate to use a certain spectrum of values of the parameter r_0. All variables related to the moving particles are eliminated inside the sphere. In particular, the Fourier transform of the interaction of the beam particle with the entire crystal must contain a cutoff parameter r_0:

$$\sigma_f(k_\perp) = 4\pi Z_1 Z_2 e^2 \int_{r_0}^{\infty} e^{-\varkappa s} \frac{\sin k_\perp s}{k_\perp s} s\, ds. \tag{8}$$

Substituting (8) into expression (4), we arrive at the basic double integral of the theory for the special function $S(R_\perp)$

$$S(R_\perp) = -4\pi Z_1 Z_2 e^2 \int_{r_0}^{\infty} e^{-\varkappa s} ds \int_0^\infty k_\perp^2 e^{-\frac{1}{2}\langle r_\perp^2\rangle k_\perp^2} J_0\left(k_\perp R_\perp \frac{n_z a_z}{|z|}\right) \sin k_\perp s\, dk_\perp. \tag{9}$$

Here we have made use of the absolute convergence of the salient integrals.

μ	$I(\mu)$
0	—0,5
1	—0,286
1,5708	—0,082
2	0,043
2,5	0,121
3	0,142
4	0,105
5	0,059
6	0,032
7,854	0,017
10	0,0103

If the function $S(R_\perp) > 0$ in the neighborhood of the center of a spot $(R_\perp \sim 0)$, the scattering intensity will, on the basis of (3), be increased over the background ($\rho_f^{(1)} > 0$) which corresponds to a Wehner spot. At the center of the spot $R_\perp = 0$, $J_0\left(k_\perp R_\perp \frac{n_z a_z}{|z|}\right) = 1$, and the inner integral in (9) is reduced to the special function $I(\mu)$:

$$\int_0^\infty k_\perp^2 e^{-\frac{1}{2}\langle r_\perp^2\rangle k_\perp^2} \sin k_\perp s\, dk_\perp = \frac{dI(\mu)}{d\mu}, \quad \left(\mu = s\left(\frac{1}{2}\langle r_\perp^2\rangle\right)^{-\frac{1}{2}}\right) \tag{10}$$

$$I(\mu) = -\int_0^\infty x e^{-x^2} \cos \mu x\, dx.$$

The asymptotic behavior of this function at large and small μ takes the form

$$I(\mu) \to \begin{cases} -\frac{1}{2}, & \text{as } \mu \to 0 \\ \frac{1}{\mu^2}, & \text{as } \mu \to \infty \end{cases}$$

The values of the function $I(\mu)$ are given in the table. It shows that $I(\mu)$ is positive for all $\mu > 1.57$, and that its derivative $I'(\mu) = dI(\mu)/d\mu$ is negative for all $\mu \geqslant 3$.

When $R_\perp = 0$, the function $S(R_\perp)$ is expressed in terms of $I'(\mu)$ as follows:

$$S(0) = -4\pi Z_1 Z_2 e^2 \left(\frac{2}{\langle r_\perp^2\rangle}\right)^{1/2} \int_{r_0\left(\frac{2}{\langle r_\perp^2\rangle}\right)^{1/2}}^{\infty} I'(\mu) \exp\left[-\left(\frac{\langle r_\perp^2\rangle}{2}\right)^{1/2} \varkappa\mu\right] d\mu. \tag{11}$$

We conclude that a sufficient condition for positiveness of $S(0)$ is

$$r_0 \geqslant 3\left(\frac{1}{2}\langle r_\perp^2\rangle\right)^{1/2}. \tag{12}$$

When (12) is satisfied, we obtain the following formula for the depth of the spot:

$$\rho_f^{(1)}(\mathbf{r}, t)\big|_{R_\perp=0} = \left(\int_{(\Omega)} \rho\, dr\right) \frac{1}{m|z|^2} \frac{a_z}{2\pi} \int_{\frac{|r|}{t}}^{\infty} \frac{1}{\xi} \Phi(\xi)\, d\xi \sum_{n_z=1}^{\nu_a} n_z S(0) > 0.$$

Thus, if forces of repulsion dominate in the forces of interaction between the beam particles and crystal atoms in the presence of impenetrable spheres around the atoms of the crystal, and if the radius of the impenetrable spheres satisfies the condition (12), what occurs is not blocking, but an increase in the intensity of the particles at the points of the collector that fall on the centers of lunes.

The change in sign of the intensity has been proven only for the center of the spot. However, the proof also remains valid in a certain neighborhood of this center with a sufficiently large radius to play a role in the experiment.

Actually, this requires that it be possible to approximate the Bessel function $J_0(k_0 R_\perp n_z a_z/|z|)$ in the integral of (9) by unity even in the regions in which its argument is nonzero. This is possible if the effective width of the other multiplier in the integrand (the Gaussian function $\exp\left[-\frac{1}{2}\langle r_\perp^2\rangle k_\perp^2\right]$) is within the first maximum of the zeroth-order Bessel function. This requires simultaneous satisfaction of two inequalities

$$\left(\frac{1}{2}\langle r_\perp^2\rangle\right)^{1/2} k_\perp > 1,$$

$$k_\perp \delta r_\perp \frac{n_z a_z}{|z|} \leqslant 2{,}405,$$

which can be done if the radius of the neighborhood around the center of the spot ($\delta r_\perp$) is small enough. We find:

$$\delta r_\perp \leqslant \left(\frac{1}{2}\langle r_\perp^2\rangle\right)^{1/2} \frac{2{,}405\,|z|}{n_z a_z}.$$

Putting $\left(\frac{1}{2}\langle r_\perp^2\rangle\right)^{1/2}/a_z \sim 10^{-1}$, $|z| \sim 10$ cm, and $n_z \sim 5$, we obtain $\delta r_\perp \leqslant 0.5$ cm, which is sufficient to play an appreciable role in experiments.

In the other limit $r_0 = 0$, we have

$$S(R_\perp) \equiv 2\pi Z_1 Z_2 e^2 \varkappa^2 S(a, X, 0);$$

$$S(a, X, 0) = -\frac{1}{2} e^{-\frac{X^2}{4a}} + e^a \int_a^\infty e^{-t-\frac{X^2}{4t}} \frac{dt}{t}; \quad a = \frac{1}{2}\langle r_\perp^2\rangle \varkappa^2;$$

$$X = R_\perp \frac{n_z a_z}{|z|}\varkappa = \left| \mathbf{r}_\perp + (m_x \mathbf{a}_x + m_y \mathbf{a}_y) \frac{|z|}{n_z a_z} \right| \cdot \frac{n_z a_z}{|z|}\varkappa.$$

This function was investigated in [8]. Its asymptotic behavior in the neighborhood of the center and on the periphery of the spot is

$$S(a, X, 0) \to \begin{cases} -\frac{1}{a^2} e^{-\frac{X^2}{4a}} & \text{as } X \to 0 \\ 2e^a K_0(X) & \text{as } X \to \infty \end{cases}.$$

where $K_0(t)$ is a Macdonald function. In this case, the function $S(R_\perp)$ describes the "lune" with a halo, that is characteristic for the blocking of ions. In particular, $S(0) < 0$ in contrast to the preceding case.

In sum, we arrive at the conclusion that Wehner spots in a repulsive potential change to blocking lunes, at least in the neighborhood of their centers, on a change in the radius of the impenetrable spheres, which depends on the kinetic energy of the moving particles, r_0 passes through the critical value $r_0 \sim 3\left(\frac{1}{2}\langle r_\perp^2\rangle\right)^{1/2}$. In either case, the statistical mechanism of particle translation through the crystal is wholly preserved.

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