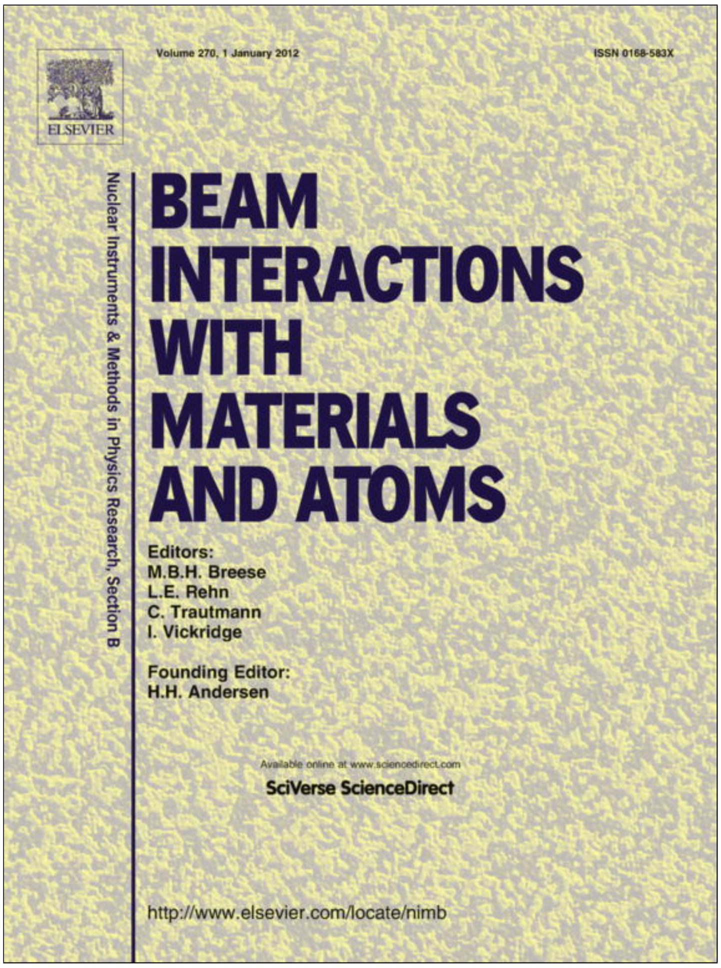

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Resonant coherent excitation of ions in planar channel of crystal with inclined beam incidence

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ABSTRACT

Resonant coherent excitation of relativistic heavy ions in crystals under planar channeling conditions is considered at beam incidence inclined with respect to the channeling plane. The beam inclination leads to effective exclusion of contribution of ions with small energy of transverse motion from observables of resonant coherent excitation. This effect can be used for resolution of the observables by individual ion trajectories.

1. Introduction

Resonant coherent excitation of ions in monocrystals (RCE or Okorokov effect) occurs when periodic electric field inside a crystal acts resonantly on some electron transition in electron cloud of the moving ion (see the review [1] and references therein). Experimentally, RCE can be detected by observing resonant changes in charge-state distribution of ions passed through a target, caused by enhanced ionization of RCE-excited ions. Another way of observation is registration of characteristic X-ray radiation emitted by resonantly excited ions. The first reliable observations of RCE were performed under conditions of axial [2] and, later, planar [3] channeling by S. Datz's group. A series of interesting experiments on RCE of relativistic heavy ions under planar channeling conditions and without channeling was performed over the last 12 years [4–11].

Under axial channeling, tuning on a resonance is achieved by changing energy of ions [2]. In the case of planar channeling, the resonance can be scanned by rotating the target in the channeling plane, that is more convenient from the experimental point of view [3,4]. In this case the ions entered the target with various impact parameters move then along curvilinear trajectories, being repelled by channel walls [12]. Neglecting multiple elastic collisions of the ion with target electrons and nuclei, we can assume that ion trajectory is unambiguously determined by its impact parameter. Thus the ion motion is oscillating around a channel center, while amplitude of these oscillations is determined by the impact parameter, which is a value of ion transverse coordinate at the moment when it enters the target [14].

Characteristics of processes, leading to excitation and subsequent ionization of the ion during RCE at each moment of time, depend on its transverse coordinate in the channel in that moment. So amplitude of a resonant electric field, ionization rate and Stark splitting of excited levels of the ion caused by Lindhard potential grow upon approaching the channel walls [4]. Therefore ions with larger amplitudes of transverse oscillations in the channel undergo more intense RCE process [5].

All ions, entered the channel with various impact parameters, contribute to the observable characteristics of RCE (e.g., charge distribution and characteristics of X-ray radiation). As a result, resonant profiles of survival fraction (i.e., fraction of ions retained their charge state after passing through the target) and X-ray yield have a rather complex structure reflecting contributions of ions with various trajectories [6,7].

For theoretical description of RCE of multiply-charged ions, density matrix formalism, allowing to describe interplay of coherent and incoherent processes in electron clouds of the ions, was developed and successfully used [15–18] (alternative methods for theoretical description of RCE are presented in [19–21]). This approach allowed to calculate both charge-state distributions of ions and properties of characteristic X-ray radiation observed during RCE. In order to reproduce experimentally observed resonant profiles of survival fraction and X-rays yield, the model of *coherence zone*, allowing to take into account intense incoherent processes near channel walls, have been introduced into the density matrix formalism. In this model we assume that a resonant

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contribution to RCE observables is provided only by the ions with amplitudes of transverse motion restricted to some zone near the channel center.

For better understanding of the role of incoherent processes at different distances from the channel center during RCE under planar channeling and for further development of the coherence zone model, resolution of contributions to RCE observables, given by ions with different trajectories, is desirable. One method to achieve such resolution, realized experimentally in [10], is based on RCE in very thin target with a thickness corresponding to a quarter-period of ion transverse oscillations in the channel. Registration of ions, emerged from the target at different angles to the channeling plane, unambiguously determined by their impact parameters, allowed to identify their trajectories. Another way to resolve RCE observables over ion trajectories relies on registration of the passed ions and X-ray photons in coincidence with energy, transferred from ions to the target in a process of their deceleration. Such kind of experiments were performed in [5].

In this article, we propose a new method of experimental realization of ion-trajectory resolution of RCE observables based on inclination of the ion beam with respect to the channeling plane. It is shown that the beam inclination leads to exclusion of the ions with impact parameters fitting into some region near the channel center from the RCE process; size of this region depends on an inclination angle. Our calculations are aimed on description of the experimental data [4] on hydrogen-like ions Ar^{17+} with energy 390 MeV/u propagating in the channel $(2\bar{2}0)$ of Si crystals with 94.7 μm thickness.

The rest of this article is organized as follows. Is Section 2 we formulate the density matrix approach and the model of coherence zone. The method of trajectory resolution of RCE observables based on inclination of the beam is described in Section 3. Results of calculations illustrating this method are presented in Section 4, and conclusions are formulated in Section 5.

2. Density matrix approach

To begin with, we will briefly describe the approach, based on density matrix formalism and coherence zone model, and used to for simulation of RCE at planar channeling [15–18]. We characterize quantum state of bound electrons of the ion by the density matrix ρ which evolves in time (t' – time in the ion rest frame) according to the Master equation [22]

$$i\frac{d\rho}{dt'} = [H,\rho] + R(\rho), \tag{1}$$

where the Hamiltonian $H = H_0 + \sum_{i=1}^{N} V_i$ is a sum of the free ion Hamiltonian H_0 and operators of interaction $V_i = -e\varphi(\mathbf{r}_i) + (e/2mc)(\mathbf{p}_i\mathbf{A}(\mathbf{r}_i) + \mathbf{A}(\mathbf{r}_i)\mathbf{p}_i)$ of each of N bound electrons of the ion with scalar φ and vector $\mathbf{A}$ potentials of electromagnetic field of the crystal arising in the reference frame of the moving ion. The operator R is responsible for relaxation (incoherent) processes – in our case, ionization by impacts with electrons of the target and spontaneous decay of ion excited. Explicit expressions for H and R can be found elsewhere [16–18].

The Eq. (1) is solved repeatedly for each ion ensemble, moving along its individual trajectory in the channel. The operators H and R, entering this equation, depend on transverse coordinate of the ion in the channel. In the laboratory frame, the ion transverse motion obeys the equation (t is time in this frame)

$$\gamma M\frac{d^2 z_{\rm ion}}{dt^2} = -e(Z-N)V'_{\rm L}(z_{\rm ion}), \tag{2}$$

where $z_{\rm ion}$ is transverse coordinate of the ion, measured from the channel center, M and Z are ion mass and charge of its nucleus, $\gamma = (1 - v_{\rm ion}^2/c^2)^{-1/2}$ is the Lorentz factor, $v_{\rm ion}$ is a velocity of ion motion along the channel. The continuous Lindhard potential $V_{\rm L}(z)$ keeps the ion inside the channel and can be represented in-crystal electric field, averaged along the channel direction [12].

Solving the Eqs. (1) and (2) for each value of the impact parameter $z_{\rm in}$ (i.e., ion transverse coordinate $z_{\rm ion}$ at the moment of entering into the target) within the interval $-d/2 < z_{\rm in} < d/2$ (d is the channel width), we get the time-dependent density matrix $\rho(t, z_{\rm in})$. In our example, we write down the density matrix ρ in a basis of stationary states of unperturbed hydrogen-like ion Ar^{17+}. In such approach, its trace at the moment of leaving the target $t_{\rm out}$ is a fraction of hydrogen-like ions remaining after passing through the target and avoided ionization inside: $n(z_{\rm in}) = {\rm Tr}[\rho(t_{\rm out}, z_{\rm in})]$.

The main characteristic of RCE, measured in experiments [2–7,9–11] is the survival fraction f, equal to a fraction of non-ionized ions in the beam after passing through the target. It can be obtained from $n(z_{\rm in})$ by integrating on impact parameter: $f = \frac{1}{d}\int_{-d/2}^{d/2} n(z_{\rm in})dz_{\rm in}$. Characteristics of X-ray radiation, emitted by ions (yield, angular distribution, polarization) can be obtained by using a similar averaging procedure [16,17,23].

According to the coherence zone model, we assume that intense incoherent processes outside the coherence zone with a half-width $z_{\rm max}$ suppress RCE. Thus we exclude the periodic field which coherently excites the ion from Eq. (1) at $|z_{\rm in}| > z_{\rm max}$, obtaining the density matrix $\rho^{\rm (bk)}$ corresponding to a non-resonant background. In this case, a fraction of ions retained their initial charge state on exit from the target is $n^{\rm (bk)}(z_{\rm in}) = {\rm Tr}\left[\rho^{\rm (bk)}(t_{\rm out}, z_{\rm in})\right]$. To exclude contribution of non-resonant processes from the survival fraction, we subtract its non-resonant background value. The result is a purely resonant contribution to the survival fraction:

$$\Delta f = \frac{1}{d}\int_{-z_{\rm max}}^{z_{\rm max}} \Delta n(z_{\rm in})dz_{\rm in}, \tag{3}$$

where $\Delta n(z_{\rm in}) = n(z_{\rm in}) - n^{\rm (bk)}(z_{\rm in})$. Thus, ions not fitting inside the coherence zone $|z_{\rm in}| < z_{\rm max}$ do not contribute to (3).

3. Inclined beam

Consider a situation when the ion beam enters the crystal at small angle ϕ with respect to the channeling plane. As known, channeling conditions are violated when the beam incidence angle exceeds a Lindhard critical angle [12]. In the conditions under consideration [4] (390 MeV/u Ar^{17+} ions in the $(2\bar{2}0)$ channel of Si crystal) the critical angle is about 1.5×10^{-4}, so we will consider even smaller incidence angles ϕ.

An ion, entered the target at the incidence angle ϕ with the initial transverse coordinate $z_{\rm in}$ has a following energy of transverse motion:

$$E(z_{\rm in}) = \frac{\gamma M v_{\rm ion}^2 \phi^2}{2} + e(Z-N)V_{\rm L}(z_{\rm in}). \tag{4}$$

Classical turning point of transverse motion $z_{\rm t}[z_{\rm in}]$, corresponding to the impact parameter $z_{\rm in}$, should obey the equation $E(z_{\rm in}) = e(Z-N)V_{\rm L}(z_{\rm t})$. A turning point $z_{\rm t}$ (for definiteness we will take this value positive) determines an amplitude of transverse oscillations of the ion in the channel, as shown in Fig. 1. If it does not exist, then an energy of transverse motion is sufficiently large to reach channel wall – in this case dechanneling of the ion will be very probable [13].

We will follow the model of coherence zone during simulation of RCE with inclined beam as well. According to this model, we should neglect contribution to Δf, coming from ions with amplitudes of transverse motion $z_{\rm t} > z_{\rm max}$ exceeding the boundaries of the coherence zone. The ions contributing to Δf should have

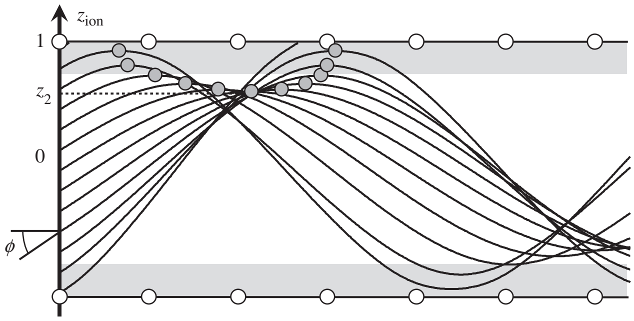

Fig. 1. Schematic view of ion trajectories in the channel with incident beam, inclined on angle ϕ. Turning points of transverse ion motion with coordinates $z_t > z_2$ are shown by gray circles. Ion trajectories, contributing to RCE, should not touch light-gray regions outside the coherence zone.

amplitude of oscillations $z_t < z_{max}$. At each given ϕ, such range of z_t corresponds to a range of impact parameters $z_{in} < z_1$, where the half-width of the "effective coherence zone" z_1 can be determined from the equation $z_t[z_1] = z_{max}$ or

$$E(z_1) = e(Z - N)V_L(z_{max}) \tag{5}$$

(in other words, z_1 is impact parameter of trajectory with amplitude reaching exactly the coherence zone boundary).

Therefore, when the beam incidence angle is ϕ, the expression (3) for resonant contribution of survival fraction should be replaced by

$$\Delta f_\phi = \frac{1}{d}\int_{-z_1}^{z_1} \Delta n_\phi(z_{in}) dz_{in}. \tag{6}$$

Here Δn_ϕ is calculated with inclined beam incidence.

Note that, since transverse motion of ions in the channel has a character of one-dimensional oscillations, inclined beam incidence gives some nonzero initial velocity to this motion and thus leads to increase of its amplitude and shift of its phase (in comparison with the case of normal incidence). At large thickness of the target (we consider the case of 94.7 μm-thick Si target [4]), when an ion performs many cycles of transverse oscillations, the phase shift does not play any important role. Therefore the beam inclination leads mainly to effective enlargement of ion oscillations amplitude. This allows us to set the quantity $\Delta n_\phi(z_{in})$, calculated along ion trajectory starting with inclined beam incidence, equal to $\Delta n_{\phi=0}(z_t[z_{in}])$, calculated along trajectory starting with normal beam incidence but with the same amplitude of transverse oscillations.

Calculating resonant contribution to survival fraction (6) with inclined beam, we take the region of impact parameters $|z_{in}| < z_1$ corresponding to ion trajectories located entirely in the coherence zone. The mapping $z_t[z_{in}]$ converts this region of impact parameters to a region of turning points (or region of oscillation amplitudes) $z_2 < z_t < z_{max}$ (see Fig. 1). The lower boundary of this region z_2 is determined by ions with the smallest energy of transverse motion, possible at inclined beam incidence (i.e., ions with the impact parameter $z_{in} = 0$ fitting into the minimum of the Lindhard potential): $z_2 = z_t[0]$ or

$$E(0) = e(Z - N)V_L(z_2). \tag{7}$$

Using the mapping $z_t[z_{in}]$, we can express the resonant contribution to the survival fraction (6) obtained with inclined beam in terms of quantities $\Delta n_{\phi=0}$, calculated at normal incidence:

$$\Delta f_\phi = \frac{2}{d}\int_0^{z_1} \Delta n_\phi(z_{in}) dz_{in} = \frac{2}{d}\int_{z_2}^{z_{max}} \Delta n_{\phi=0}(z_t)\frac{dz_{in}}{dz_t} dz_t. \tag{8}$$

If we approximate the Jacobian dz_{in}/dz_t by a ratio of the integration ranges $z_1/(z_{max} - z_2)$, Eq. (8) will take the simpler form:

$$\Delta f_\phi \approx \frac{z_1}{z_{max} - z_2}\frac{2}{d}\int_{z_2}^{z_{max}} \Delta n_{\phi=0}(z_t) dz_t. \tag{9}$$

Compare (9) with the expression for normal incidence (3), which can be rewritten as:

$$\Delta f_{\phi=0} = \frac{2}{d}\int_0^{z_{max}} \Delta n_{\phi=0}(z_t) dz_t. \tag{10}$$

As seen, inclination of the beam leads to: (a) change of Δf dependence by absolute value in comparison to the case of normal incidence, and to (b) effective exclusion of contributions of ions with small impact parameters $|z_{in}| < z_2$. The last effect arises since the beam inclination increases transverse energy (4) of all ions and thus excludes some part of the ions with small transverse energies existing at normal incidence.

By analogy with (9), expressions for other observables of RCE (yield, angular distribution and polarization of characteristic X-rays or Auger electrons, yield of metastable ions, etc.) can be obtained. Varying an inclination angle ϕ in experiments, one can change z_2 from zero to the maximal value z_{max} and thus smoothly vary a region of impact parameters contributing to observables from vanishingly narrow to maximally wide. This will allow to separate contributions of ions with different trajectories to observables of a type of (3).

The practical recipe for such trajectory resolution of the observables can be the following. First, we will need the Lindhard potential $V_L(z)$ either calculated numerically (using, e.g., Doyle–Turner potentials [24]) or extracted from channeling experiments data (see, e.g., [25]). The next step is estimation of the coherence zone half-width z_{max}, which can be found by fitting theoretically calculated survival fraction resonant profiles to experimental ones at normal beam incidence (in a manner of the works [15–17]). Another independent way to estimate z_{max} is to find experimentally such an inclination angle ϕ_{max} that $\Delta f_\phi = 0$ at any $\phi \geqslant \phi_{max}$ (i.e., at inclination angles exceeding ϕ_{max}, resonance dips in survival fraction disappear leaving only a nonresonant background). At this "RCE critical angle" $\phi = \phi_{max}, z_1 = 0$ and $z_2 = z_{max}$, so, according to (4), (5) and (7), we can find z_{max} from the following equation:

$$e(Z - N)[V_L(z_{max}) - V_L(0)] = \frac{\gamma M v_{ion}^2 \phi_{max}^2}{2}. \tag{11}$$

If we obtained experimentally the survival fraction resonant profiles Δf_ϕ for two inclination angles ϕ_1 and $\phi_2 > \phi_1$, then, according to (9), we can find a trajectory resolved resonant contribution to survival fraction integrated in some narrow range of impact parameters:

$$\frac{2}{d}\int_{z_2^{(1)}}^{z_2^{(2)}} \Delta n_0(z) dz = \frac{z_1^{(1)}\Delta f_{\phi_1}}{z_{max} - z_2^{(1)}} - \frac{z_1^{(2)}\Delta f_{\phi_2}}{z_{max} - z_2^{(2)}}. \tag{12}$$

Here the quantities $z_{1,2}^{(1)}$ and $z_{1,2}^{(2)}$ can be calculated using given $V_L(z), z_{max}$ and Eqs. (4), (5) and (7) for $\phi = \phi_1$ and $\phi = \phi_2$, respectively.

Having Δf_ϕ measured at several different values of inclination angle ϕ, we can calculate trajectory resolved data (12) distributed among different integration ranges. By gradual increase of ϕ we can trace change of the trajectory resolved survival fraction upon approach to the coherence zone boundary.

4. Results

To illustrate the proposed method of trajectory resolution of RCE observables, we present calculation results for resonant contribution to survival fraction Δf_ϕ under conditions of the experiment in Ref. [4], where hydrogen-like Ar^{17+} ions with energy 390 MeV/u pass through planar $(2\bar{2}0)$ channel of Si crystal with

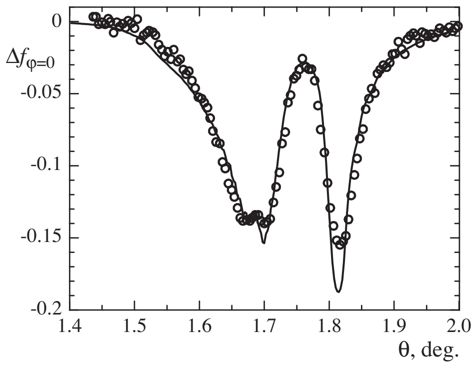

Fig. 2. Resonant contribution to survival fraction $\Delta f_{\phi=0}$ at normal beam incidence as a function of angle θ between the beam and the $[001]$ crystal axis, measured experimentally [4] (white circles) and calculated theoretically (solid line) with the coherence zone half-width $z_{\max} = 0.9\,(d/2)$; the theoretical result is additionally multiplied by 0.43.

thickness 94.7 μm. In this experiment, a scanning of resonant profile of survival fraction is performed by changing an angle θ between the beam and the crystallographic axis $[110]$. The resonance condition [4]

$$\frac{2\pi\gamma v_{\text{ion}}}{a}\left(k\sqrt{2}\cos\theta + l\sin\theta\right) = E_{\text{trans}} \qquad (13)$$

(a is the lattice constant of Si, $(k,l) = (1,1)$ are the indices of resonant harmonic of in-crystal field) relates the θ angle to the energy E_{trans} of transition $1s^2 \to [n=2]$ induced in the ion electron cloud.

In Fig. 2, experimental data from Ref. [4] for resonant contribution to survival fraction for the case of normal beam incidence $\Delta f_{\phi=0}$ as a function of θ are presented in comparison with results of our calculations. The triply split resonant dip corresponds to electron transition from the 1s state to the states $n = 2$. The left and central dips correspond to excitation of the 2s and $2p_{1/2}$ states, mixed by the Lindhard potential, whereas the right dip corresponds to excitation of almost purely the $2p_{3/2}$ state.

The results for $\Delta f_{\phi=0}$, calculated according to the formula (10), are presented for the value of coherence zone half-width $z_{\max} = 0.9\,(d/2)$. In addition, the calculated function $\Delta f_{\phi=0}(\theta)$ was multiplied by the factor 0.43. Although the experimental data and calculation results do not agree by absolute value (which can be a signature of some additional ionization processes in the target, not taken into account in our approach), agreement of resonant dip shapes is very good.

Good reproduction of the experimental data with our model at normal beam incidence allows us to use this model to predict results, which could be measured in experiments with inclined beams. Results of this prediction can be used to verify the method of trajectory resolution of observables, proposed in the previous section.

Resonant contributions to survival fraction Δf_ϕ with inclined beam incidence at different angles ϕ calculated in the framework of the coherence zone model using Eq. (6) are shown in Fig. 3 (solid lines). The values of $z_{\max}$ and additional multiplier taken here are the same as in Fig. 2. For the presented angles $\phi = 0.3\times 10^{-4}, 0.6\times10^{-4}, 0.9\times10^{-4}$ and 1.2×10^{-4} radians, the values of z_1 are, respectively, $0.89, 0.85, 0.77$ and 0.62 in the units of $d/2$, whereas z_2 is $0.20, 0.41, 0.60$ and 0.76 in the same units.

Dashed lines in Fig. 3 show the quantities Δf_ϕ calculated according to Eq. (9), i.e., by reducing the case of inclined beam incidence to the case of the normal incidence, but with a new region of impact parameters – with a part near the channel center excluded. As seen on the figure, the solid and dashed lines almost coincide, which indicates correctness of the proposed method of trajectory resolution of observables by using inclined beams.

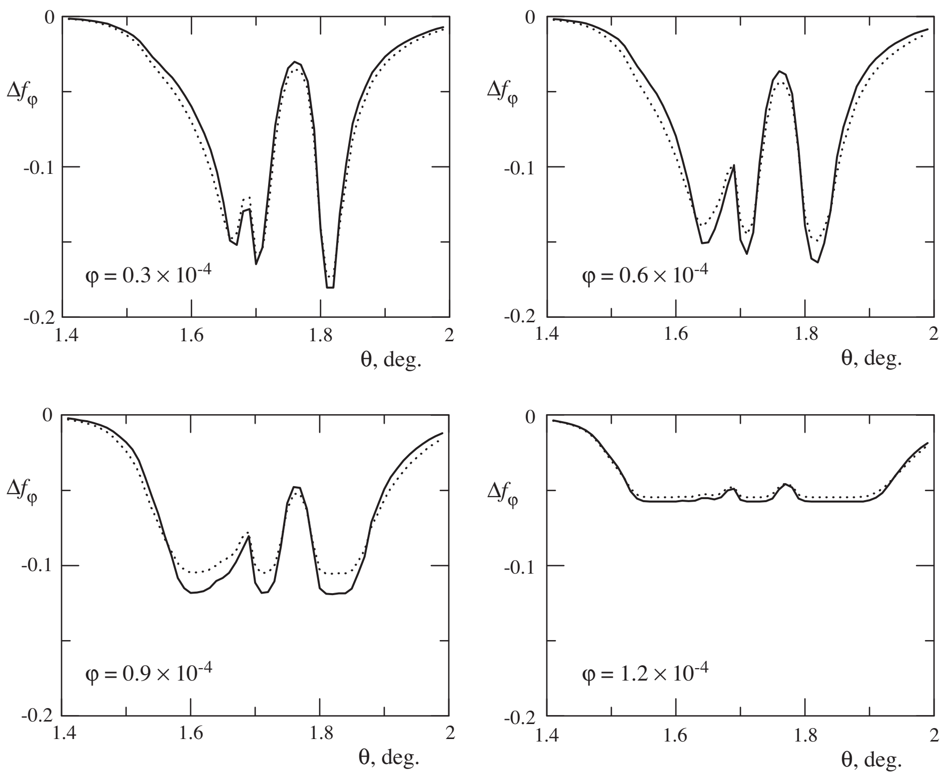

Fig. 3. Solid lines: profiles of resonant contribution to survival fraction Δf_ϕ with incident beam inclined on different angles ϕ, calculated according to (6) with $z_{\max} = 0.9\,(d/2)$ and additional multiplier 0.43. Dashed lines: profiles of Δf_ϕ calculated according to (9) by reduction to the case of normal beam incidence.

Flattening of the curves in Fig. 3 at increase of ϕ reflects growth of a mean amplitude of ion transverse oscillations in the channel, leading to increasing smearing of the resonant dips by Stark splitting of the ion excited states, which depends on ion transverse coordinate. Such a regularity conforms with effective exclusion of a part of ions with small transverse energies from RCE process, increasing with increase of ϕ.

5. Conclusions

Resonant coherent excitation of ions at planar channeling in monocrystals grants a possibility to study a lot of processes occurring with ions in oriented spatially nonuniform targets. Each ion, moving along its curvilinear trajectory in the channel, passes alternately through regions with different field amplitudes and electron densities. Ions moving along very different trajectories contribute all together to experimentally observed RCE characteristics.

Resolution of RCE observables by individual ion trajectories is important problem from the point of view of fundamental understanding of coherent and incoherent processes in channeled ions, and also for further development of the coherence zone model, successfully used for theoretical treatment of RCE.

In this article, we proposed the new method allowing to perform resolution of observables by ion trajectories and based on usage of ion beam, inclined with respect to the channeling plane. It was shown that the RCE observables obtained with inclined beam can be related to the observables obtained at normal incidence but with excluded contribution of ions from some region near the channel center. Width of this region increases with increasing beam inclination. This allows to resolve the observables by individual ion trajectories by varying an inclination angle.

Behavior of trajectory resolved survival fraction upon increase of impact parameter should reveal the physics of RCE process under planar channeling conditions. In particular, we can expect that degree of resonant suppression of survival fraction should grow with increase of impact parameter owing to growing amplitudes of resonant field of the crystal. At the coherence zone boundary, this suppression should diminish back due to strong incoherent processes near the channel walls. Besides, the usage of inclined beam offers a possibility to estimate a coherence zone width on a basis of experimental data without need of full density-matrix RCE modeling.

The proposed method was illustrated in the article by calculations of survival fraction of hydrogen-like Ar^{17+} ions under conditions of the experiment [4]. The calculation results demonstrate workability of this method.

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