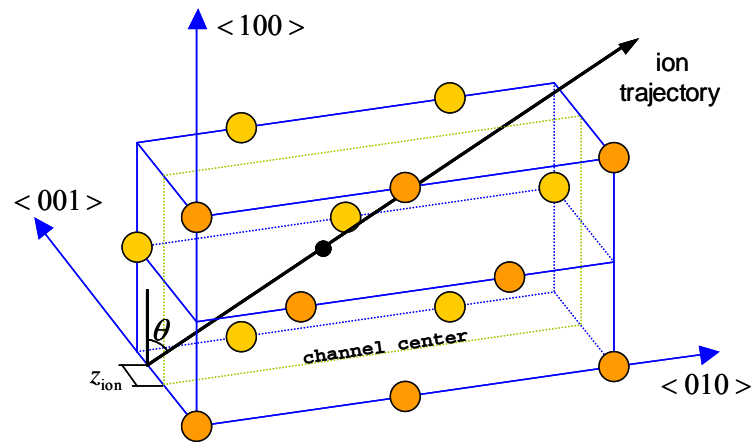


X-ray production from resonant coherent excitation of relativistic HCIs in crystals as a model for polarization XFEL studies in the keV range

V.V.Balashov, A.A.Sokolik, A.V.Stysin

D.V.Skobeltsyn Institute of Nuclear Physics, M.V.Lomonosov Moscow State University, Moscow 119991, Russia



Fourier series of the potential of the in-target electric field and its Lorentz transformation to the ion rest frame;

Scalar potential $\varphi(\vec{r})$ of the electric field of the crystal is composed in the laboratory frame into its Fourier (kln) harmonics

$$\varphi(\vec{r}) = \sum_{kln} \Phi_{kln} e^{i\vec{G}_{kln}\vec{r}},$$

with wave vectors \vec{G}_{kln} being reciprocal lattice vectors. After a set of successive coordinate frame transformations this potential is transformed into the the scalar and vector electromagnetic potentials in the ion rest frame:

$$\begin{aligned} \varphi'(\vec{r}', t') &= \gamma \sum_{kln} e^{i\omega t'(\vec{G}'_{kln})_x} \Phi_{kln} e^{\pi i n(z_{ion}/d+1/2)} e^{i\vec{G}'_{kln}\vec{r}'}, \\ \vec{A}'(\vec{r}', t') &= -\vec{e}_x \frac{\gamma v}{c} \sum_{kln} e^{i\omega t'(\vec{G}'_{kln})_x} \Phi_{kln} e^{\pi i n(z_{ion}/d+1/2)} e^{i\vec{G}'_{kln}\vec{r}'}. \end{aligned}$$

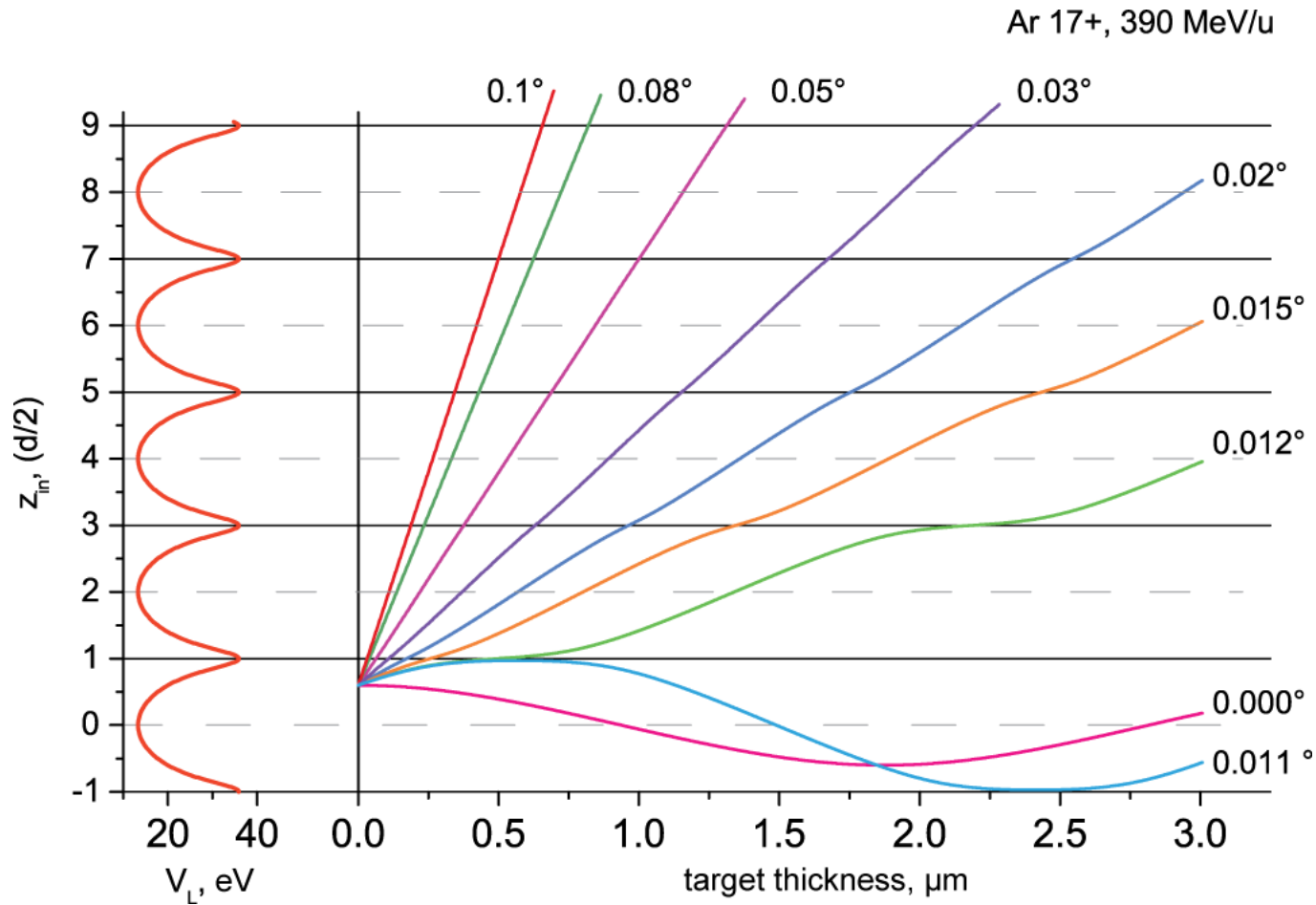
with vectors $\vec{G}'_{kln} = \vec{G}_{kln} + (\gamma - 1)(\vec{G}_{kln})_x \vec{e}_x$ standing for the reciprocal lattice vectors in the ion rest frame, which x -component is γ times larger, due to relativistic lattice contraction, than x -component of \vec{G}_{kln} . Hamiltonian H_0 of the free ion and the operator

$$V = -e\varphi' + \frac{e}{2mc}(\vec{p}\vec{A}' + \vec{A}'\vec{p})$$

of its interaction with the potentials $\varphi'(\vec{r}', t')$ and $\vec{A}'(\vec{r}', t')$ form the total Hamiltonian of the channeled ion $H = H_0 + V$ entering the generalized Master equation

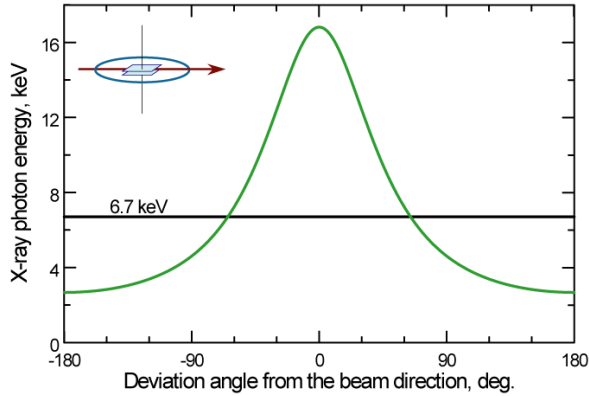
$$i \frac{\partial \rho}{\partial t} = [H, \rho] + R\rho,$$

which describes time evolution of the density matrix ρ of the ion.

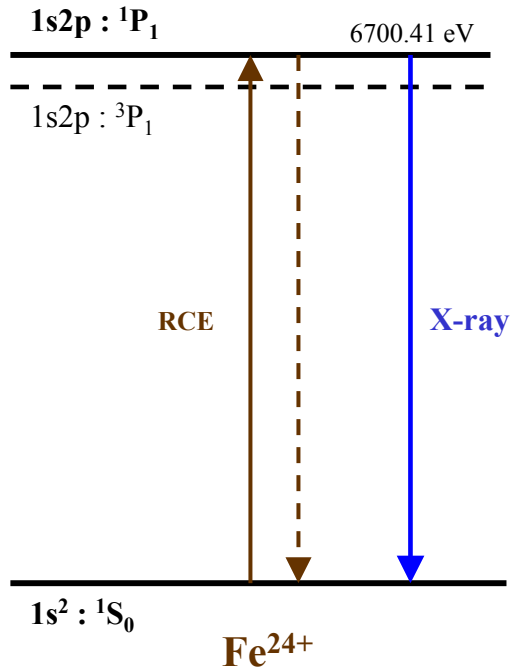


$$\Delta E = \begin{cases} \frac{2\pi\hbar}{a}\gamma v (\sqrt{2}k \cos \theta_t + l \sin \theta_t), & \text{channeling (2D);} \\ \frac{2\pi\hbar}{a}\gamma v (\sqrt{2}(k \cos \phi_t + m \sin \phi_t) \cos \theta_t + l \sin \theta_t), & \text{non-channeling (3D).} \end{cases}$$

423 MeV/u Fe²⁴⁺, 1s2p:¹P₁ → 1s²:¹S₀

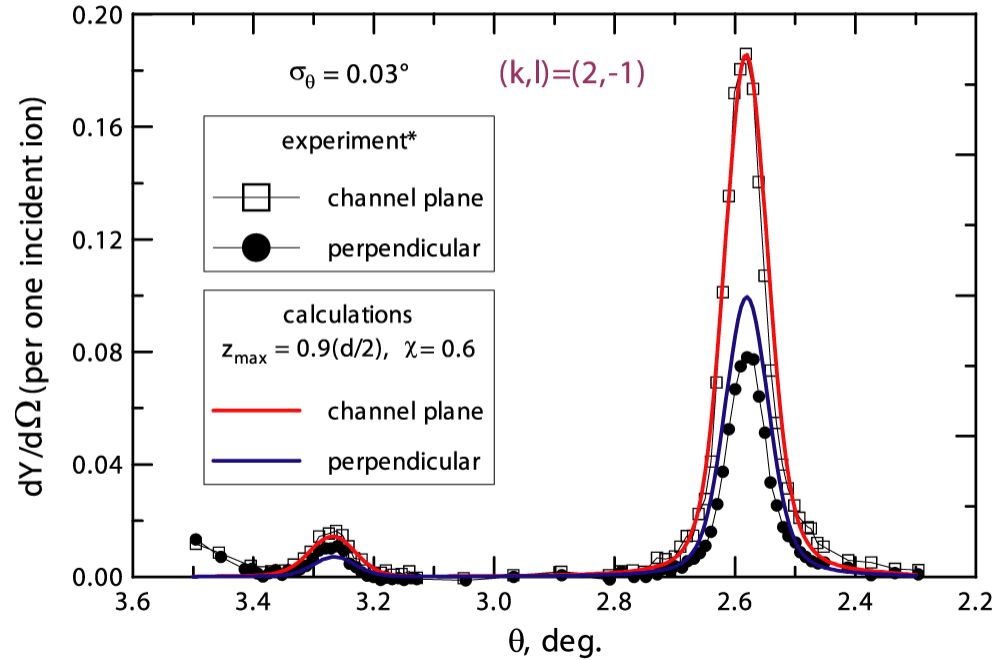


Energy range of produced photons in the lab frame:
2.67 – 16.82 keV



Anisotropic X-ray emission: experiment and calculations

423 MeV/u Fe²⁴⁺ → (2̄20) Si, thickness 21 μm



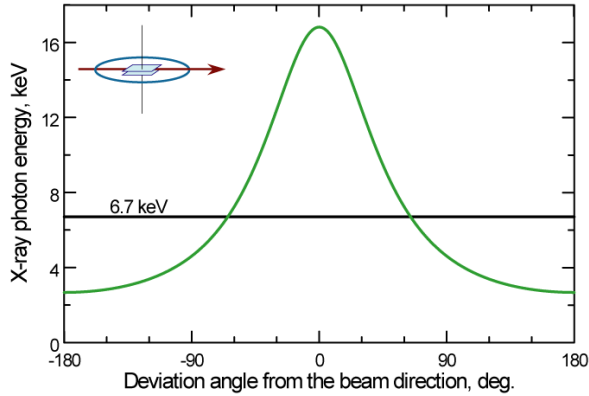
* T. Azuma, Y. Takabayashi, C. Kondo, T. Muranaka, K. Komaki, Y. Yamazaki, E. Takada, T. Murakami, Phys. Rev. Lett. 97 (2006) 145502
V.V.Balashov, A.A.Sokolik, A.V.Stysin, JETP 107 (2008) 133

Compare:

**The European XFEL
Technical Design Report**

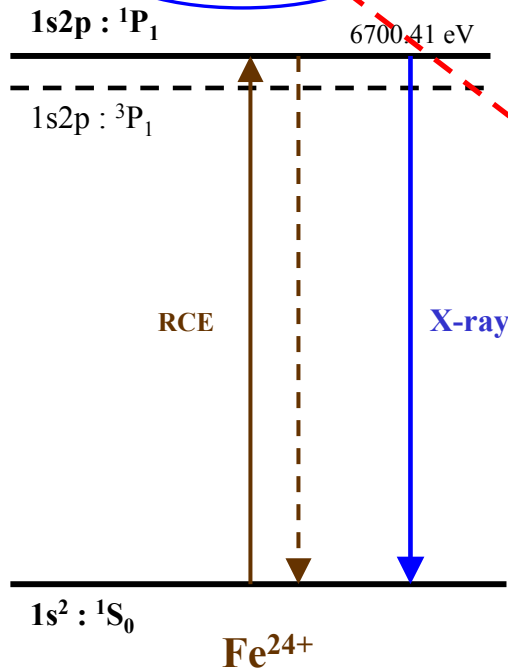
	SASE 1	SASE 2	SASE 3
Wavelengths	0.1 nm	0.1-0.4 nm	0.4-1.6 nm
Laserlike/coherent	yes	yes	yes
Polarization	linear	linear	circular, linear

423 MeV/u Fe^{24+} , $1s2p: ^1P_1 \rightarrow 1s^2: ^1S_0$



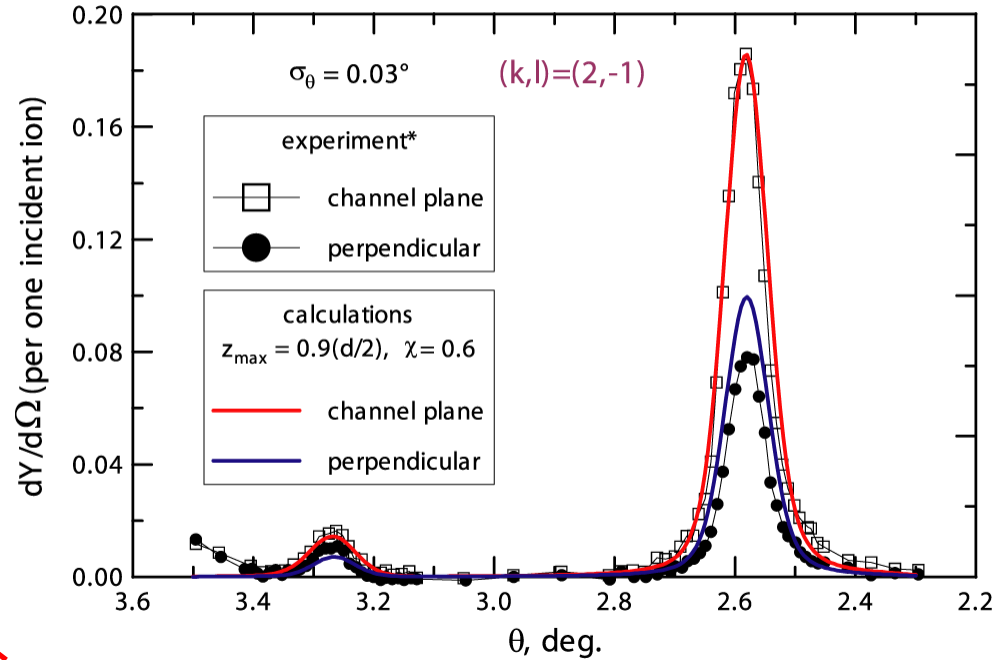
Energy range of produced photons in the lab frame:

2.67 – 16.82 keV



Anisotropic X-ray emission: experiment and calculations

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Technical Design Report

	SASE 1	SASE 2	SASE 3
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Laserlike/coherent	yes	yes	yes
Polarization	linear	linear	circular, linear

Stokes parameters of the characteristic X-ray radiation from RCE ions

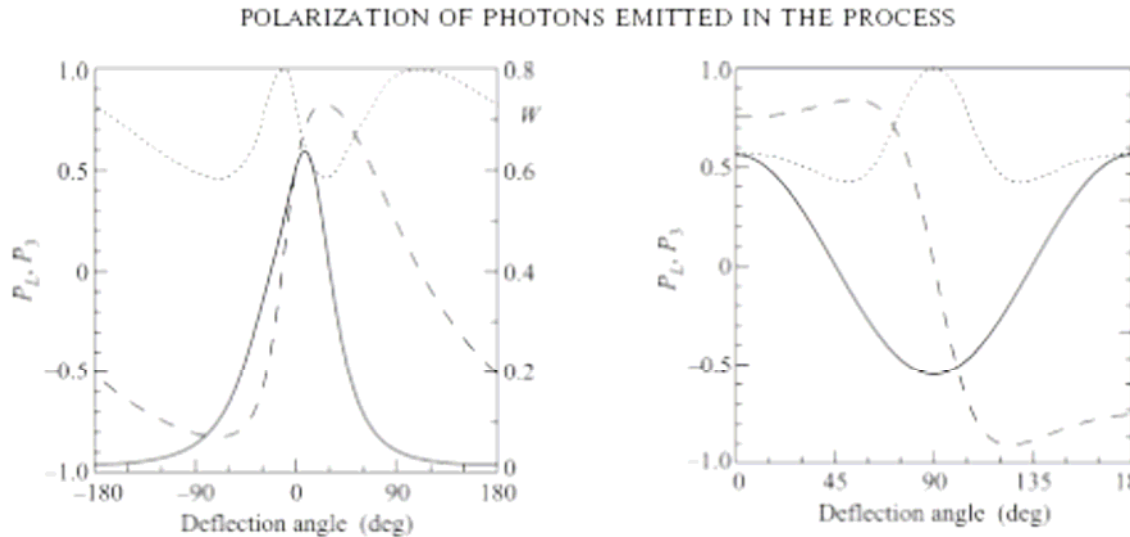


Fig. 1. Angular distributions of (solid line) the yield of photons W (in arbitrary units) and (dotted line) linear polarization degree P_L in the channeling plane in the laboratory frame as calculated under the conditions of the experiment with the 21- μm -thick target reported in [2]. (Dashed line) The circular polarization degree P_C is calculated for the 0.9- μm -thick target with averaging only over one half of the channel.

Fig. 2. Same as in Fig. 1, but in the sweep over a cone the photon deflection angle 43.5° from the ion beam in the rest frame of the ion, these photons are emitted perpendicularly to the beam).

The calculations show that since the photon yield and their polarization parameters in conditions typical or close to current RCE experiments are expected to be large, the resonance coherent excitation method can be considered as a candidate for a tunable source of polarized X-ray radiation in the keV region.

1965 – 2006 : RCE exclusively **with channeled ions** –

V.V.Okorokov, *Yad. Fiz.* 2 (1965) 1009; *Pis'ma Zh. Eksp. Teor.Fiz* 2 (1965) 175

S.Datz, C.D.Moak et al., *PRL* 40 (1978) 843; *NIM* 170 (1980) 15

K.Komaki, T.Azuma et al., *NIM B* 146 (1998) 19,
and many other.

Since 2006: RCE measurements **with both channeled ions and without channeling** at all

Present-day portrait of the RCE process (*the Okorokov effect*) from Tokyo RCE measurements of 2006-2009:

Anisotropic X-ray emission from helium-like Fe²⁴⁺ ions aligned by RCE with a periodic crystal potential –

T.Azuma et al., *PRL* 97 (2006) 145502;

Three-dimensional RCE of nonchanneling ions in a crystal –

C.Kondo et al., *PRL* 97 (2006) 135503;

Trajectory dependent RCE of planar-channeled ions in a thin Si crystal –

C.Kondo et al. *NIM B* 256 (2007) 157;

Doubly-resonant coherent excitation of HCI planar channeling in a Si crystal –

Y.Nakano et al., *J.Phys. Conf.Series* 58 (2007) 359;

Dressed atoms in flight through a periodic crystal field: X-UVU double resonances –

Y.Nakai et al., *PRL* 101 (2008) 113201;

RCE of lithium-like Li¹⁵⁺ ions in a thin Si crystal –

Y.Nakano et al., *J.Phys. Conf.Series* 163 (2009) 012094;

Polarization control in three-dimensional RCE –

Y.Nakano et al., *PRL* 102 (2009) 085502;

**A unified concept for theoretical analysis of RCE data and suggestions
for new measurements (Moscow State University; 1998-2009)**

Characteristic X-ray production in the RCE process

V.V. Balashov, I.V. Bodrenko -- *Phys.Lett. A* **352** (2006) 129

Metastable ion production in the RCE process

V.V. Balashov, I.V. Bodrenko -- *NIM B* **245** (2006) 52

Resonant coherent excitation of Ar¹⁷⁺ ions in planar channel of a silicon crystal

V.V. Balashov, A.A. Sokolik -- *Optics and Spectroscopy* **103** (2007) 761

**Angular anisotropy of characteristic X-radiation and Auger electrons
during the resonance coherent excitation of relativistic ions under planar channeling**

V.V. Balashov, A.A. Sokolik, A.V. Stysin -- *JETP* **107** (2008) 133.

**Characteristic X-ray radiation and Auger electrons from resonant coherently
excited highly charged ions under channeling**

V.V. Balashov, A.A. Sokolik, A.V. Stysin -- *NIM B* **267** (2009) 903.

**Kinetics of double resonant coherent excitation of relativistic multicharged ions
in crystals beyond the channeling conditions**

V.V. Balashov, A.A. Sokolik, A.V. Stysin -- *JETP* **108** (2009) 1010.

**Angular anisotropy of the RCE X-rays under planar channeling as manifestation
of geometrical properties of the in-crystal electric field**

V.V. Balashov, A.A. Sokolik, A.V. Stysin -- *NIM B* **267** (2009) 1772.

**Polarization of photons emitted in the process of resonant coherent excitation
of relativistic ions under planar channeling**

V.V. Balashov, V.K. Dolinov, A.A. Sokoli -- *JETP Letters* **89** (2009) 399.

**Density matrix description of resonant coherent excitations of swift highly charged
ions in oriented crystals**

V.V. Balashov, I.V. Bodrenko, V.K. Dolinov, A.A. Sokolik, A.V. Stysin --
J.Phys. Conf. Ser. **163** (2009) 012087.

**Polarization and correlation aspects of resonant coherent excitation of fast highly charged
ions in crystals**

V V Balashov -- *J. Phys.: Conf. Ser.* **212** (2010) 012028

Fast highly charged ion in matter – an open quantum system

Density matrix approach; the generalized Master equation

$$i\frac{\partial \hat{\rho}}{\partial t} = [\hat{H}, \hat{\rho}] + \hat{R} \hat{\rho};$$

for relativistic ions
wake potential is
very small

$$\hat{H} = \hat{H}_0 + \hat{V}(t); \quad \hat{V}(t) = \hat{V}^{(lattice)}(t) + \hat{V}^{(wake)}(t).$$

A system of coupled equations to solve:

$$\frac{\partial \rho_{pp}(t)}{\partial t} = 2 \cdot \sum_{q=1}^N \text{Im} [V_{pq}(t) \cdot \rho_{qp}(t)] - \lambda_p(t) \rho_{pp}(t) + \sum_{q \neq p} \lambda_{qp}(t) \rho_{qq}(t);$$

$$\begin{aligned} \frac{\partial \rho_{pq}(t)}{\partial t} = & -i \cdot \sum_{r=1}^N [V_{pr}(t) \rho_{rq}(t) - \rho_{pr}(t) V_{rq}(t)] - \\ & - \frac{1}{2} [\lambda_p(t) + \lambda_q(t) + \lambda_{pq}^{(elastic)}(t)] \rho_{pq}(t); \end{aligned}$$

$$\rho_{pq}(t=0) = \delta_{p1} \delta_{q1}.$$

From the generalized Master equation to RCE observables

- from density matrices for individual trajectories
to the averaged density matrix for the whole
ensemble of ions participating in the RCE process
and to the **survival fraction S**

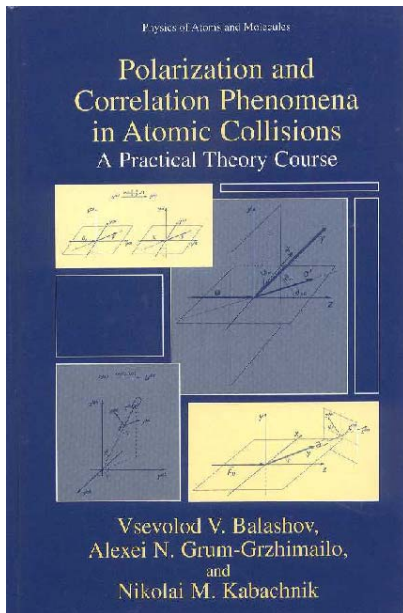
$$\langle \hat{\rho}(t) \rangle = \frac{1}{2z_{max}} \int_{-z_{max}}^{z_{max}} \hat{\rho}_{z_{in}}(t) dz_{in} \quad \longrightarrow \quad S = \text{Tr} \{ \langle \hat{\rho}(t = t_{out}) \rangle \}$$

from density matrix to statistical tensors of X-ray emitting states $\langle \hat{\rho}(t) \rangle \Rightarrow \langle \hat{\rho}(t)^{\text{rad}} \rangle \Rightarrow \langle JM | \hat{\rho}(t)^{\text{rad}} | J' M' \rangle \Rightarrow \rho_{pq}(t)$

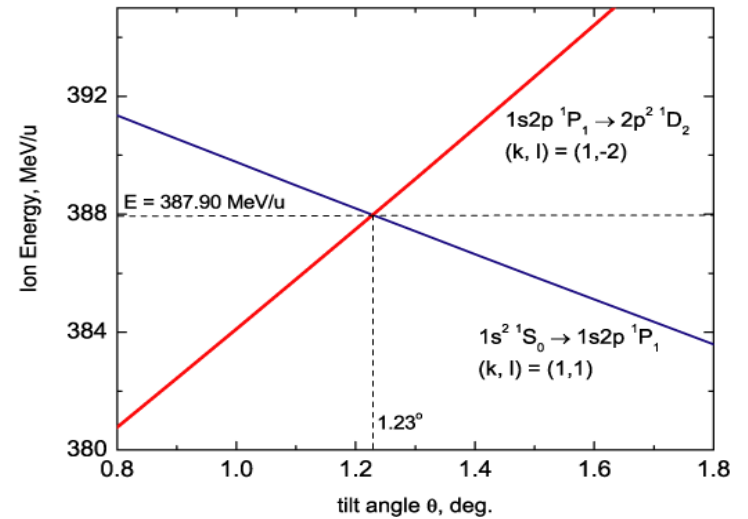
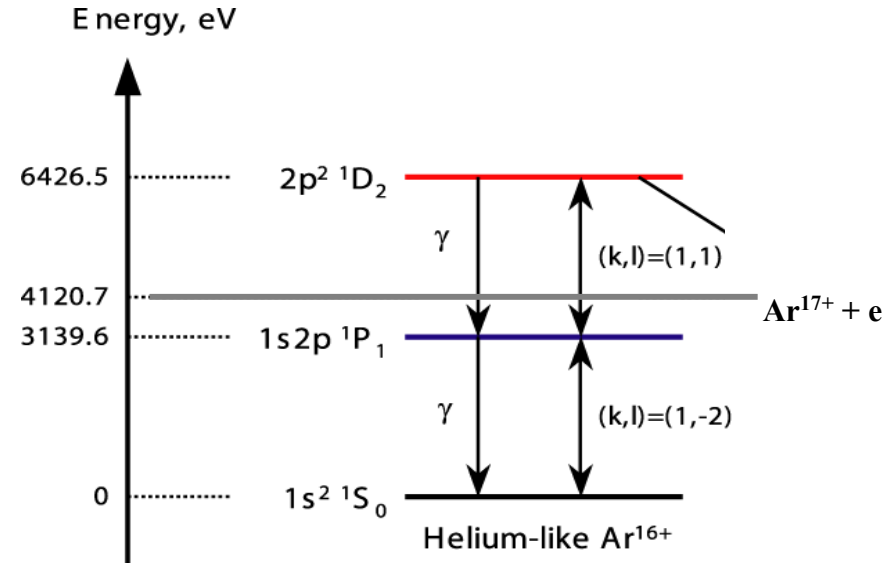
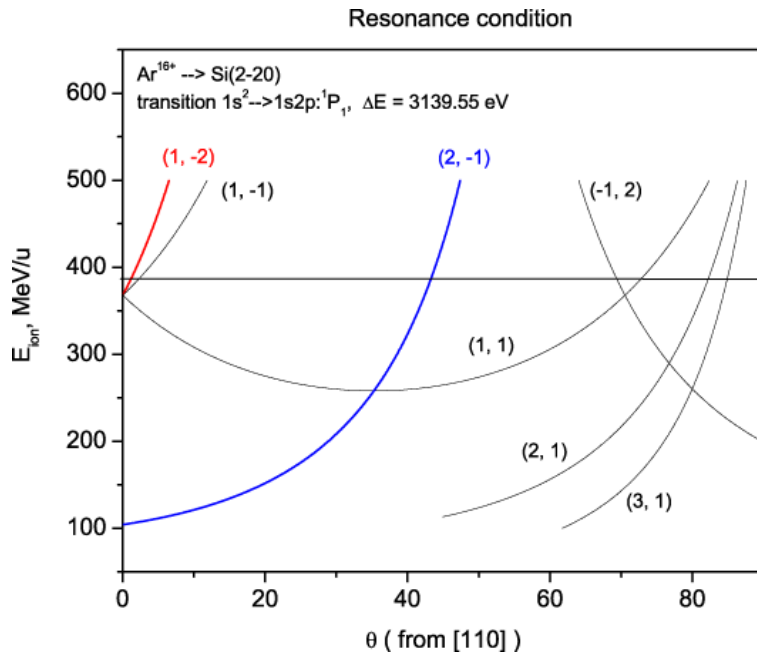
$$W_{\gamma}(\theta, \varphi) = \frac{1}{4\pi} \left[1 + \alpha_2^{\gamma} \sqrt{\frac{4\pi}{5}} \sum_{q=-2}^2 \frac{\rho_{2q}(t)}{\rho_{00}(t)} Y_{2q}(\theta, \varphi) \right]$$

The density matrix approach has shown its universality in treating the RCE process in different conditions of its observation and when performing theoretical analysis of various RCE measurements by covering, on the same theoretical ground, a wide scope of RCE observables.

This feature manifests itself especially clearly when applied to treat “two-color” excitations when two harmonics of the electric field of the crystal act on the electron cloud of the moving ion like two lasers of corresponding frequencies.



**Okorokov effect in two-colour (double resonant)
excitation of ionic autoionizing states
 Ar^{16+} (387.9 MeV/u) \rightarrow Si (220)**



Auger electrons from double RCE

Ar^{16+} (387.90 MeV/u) \rightarrow Si (220)

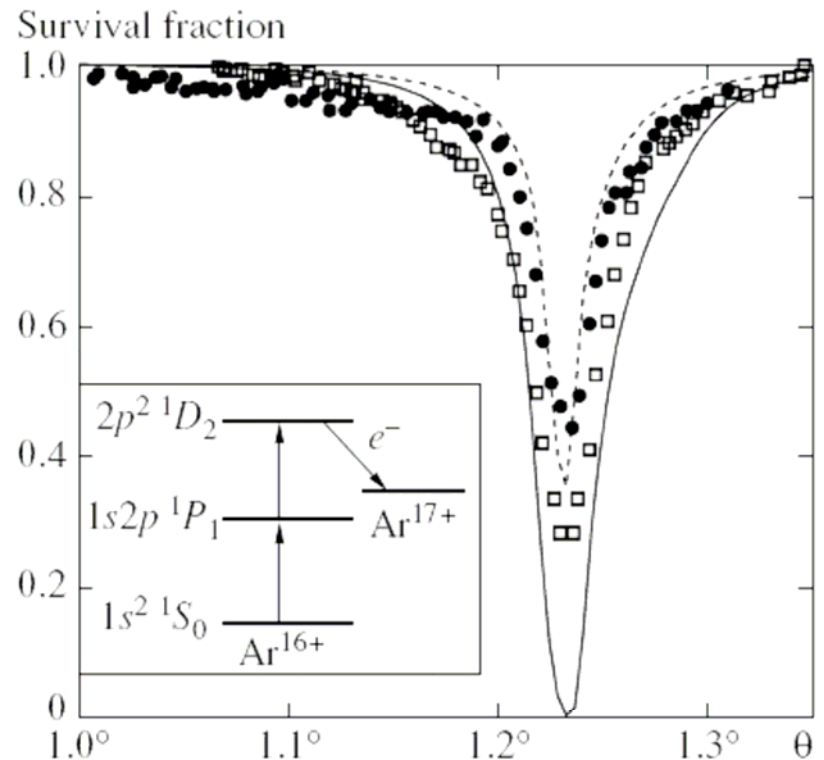
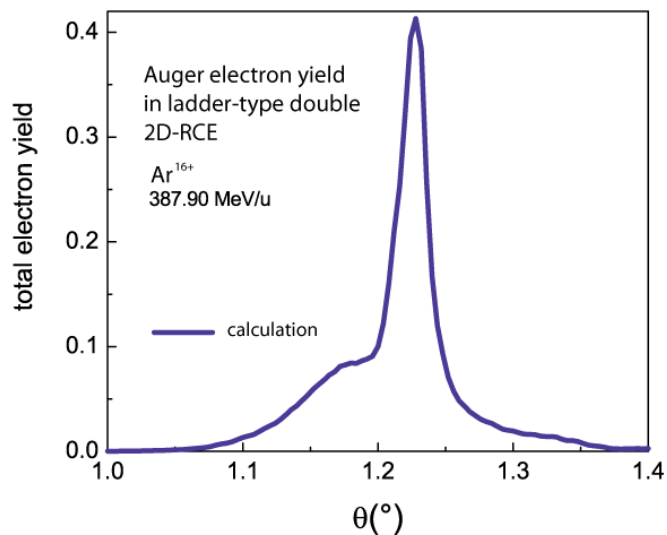
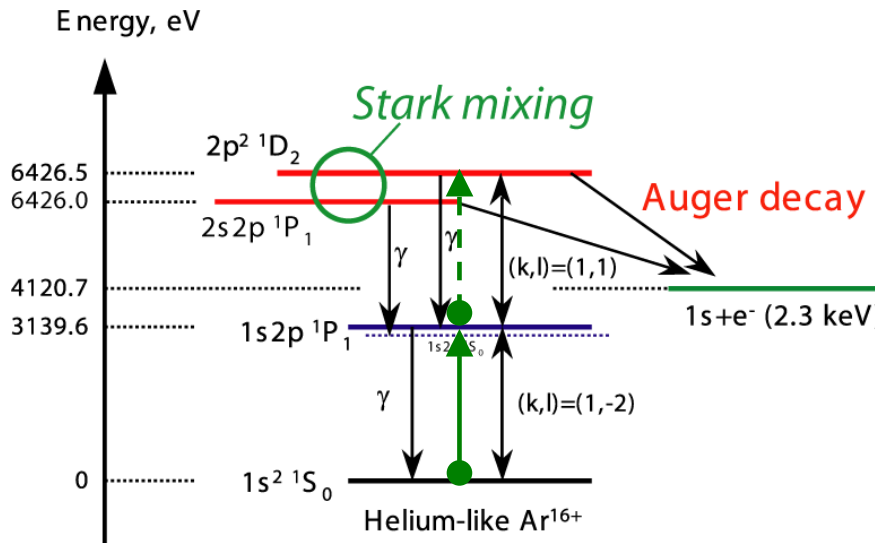
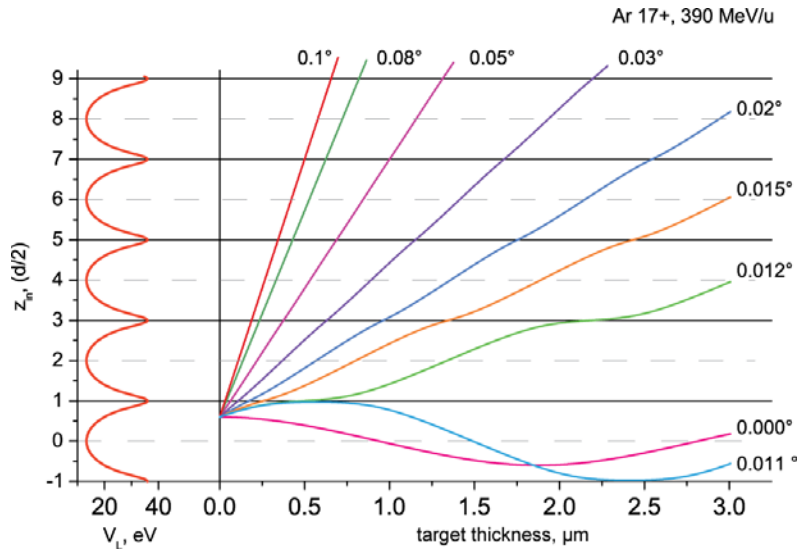


Fig. 3. Survival fraction of Ar^{16+} ions upon excitation of a single (the dashed curve is our calculation, and the circles are the experimental data from [12]) and double (the solid curve is our calculation, and the squares are the data from [12]) resonances.

RCE without channeling



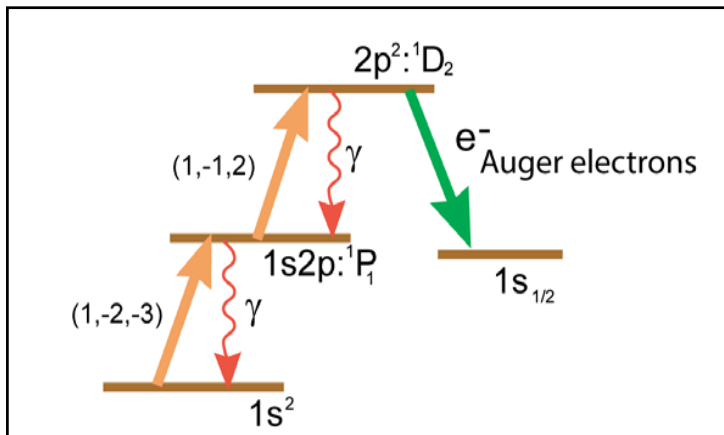
$$\begin{aligned}
 (\mathbf{G}_{klm})_x &= \frac{2\pi}{a} \left(\sqrt{2}k \cos \theta \cos \phi + l \sin \theta + \sqrt{2}m \cos \theta \sin \phi \right), \\
 (\mathbf{G}_{klm})_y &= \frac{2\pi}{a} \left(-\sqrt{2}k \sin \theta \cos \phi + l \cos \theta - \sqrt{2}m \sin \theta \sin \phi \right), \\
 (\mathbf{G}_{klm})_z &= \frac{2\pi}{a} \left(-\sqrt{2}k \sin \phi + \sqrt{2}m \cos \phi \right)
 \end{aligned}$$

$$\mathbf{E}'_{klm}(t') = -i\Phi_{klm} \left[(\mathbf{G}_{klm})_x \mathbf{e}_x + \gamma (\mathbf{G}_{klm})_y \mathbf{e}_y + \gamma (\mathbf{G}_{klm})_z \mathbf{e}_z \right] \exp(i(\mathbf{G}'_{klm})_x vt'),$$

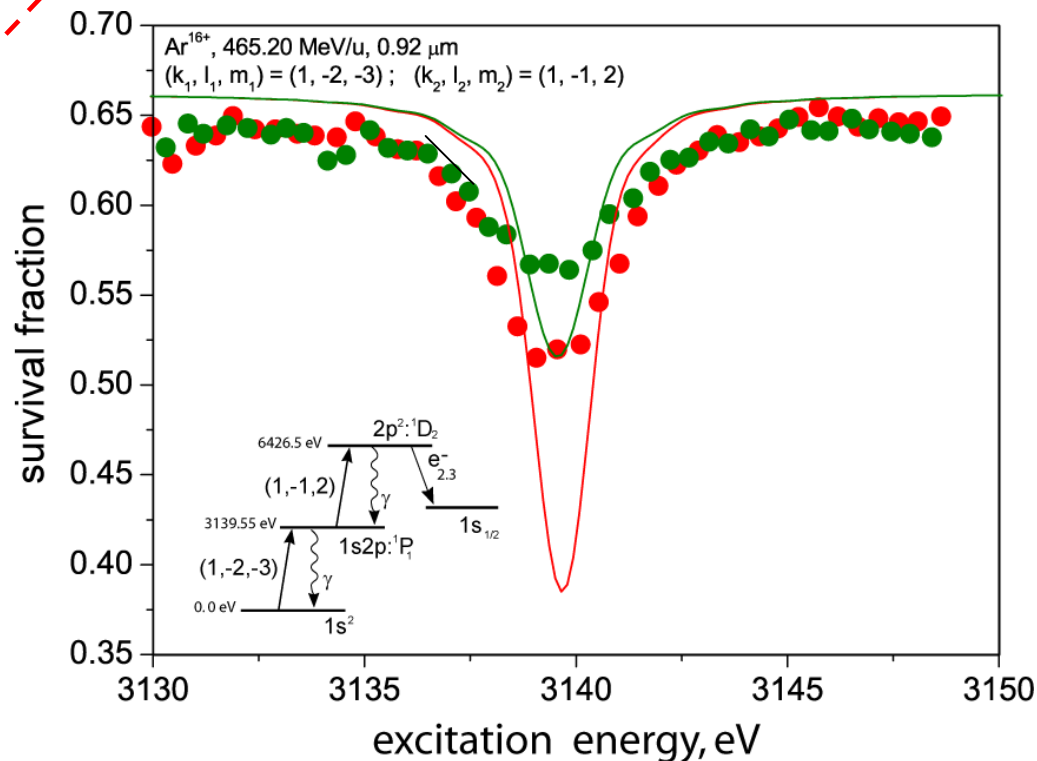
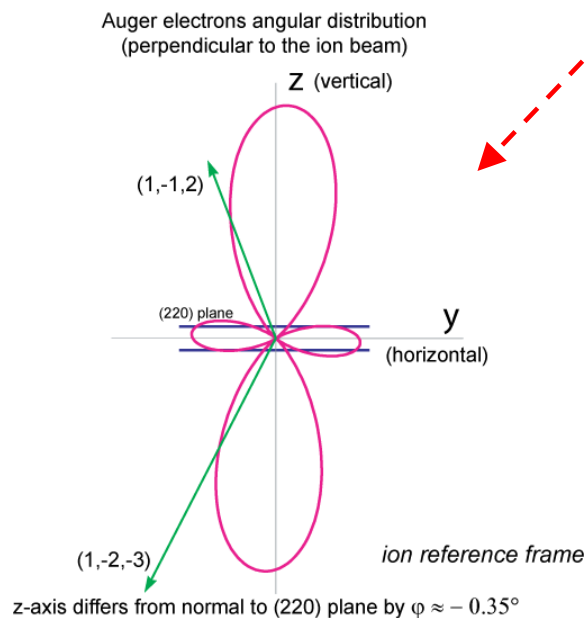
$$\begin{aligned}
 \omega_{k,l,m} &= \\
 &= \frac{2\pi\hbar}{a} \gamma v \left(\sqrt{2}(k \cos \phi + m \sin \phi) \cos \theta + l \sin \theta \right)
 \end{aligned}$$

out of the plane !

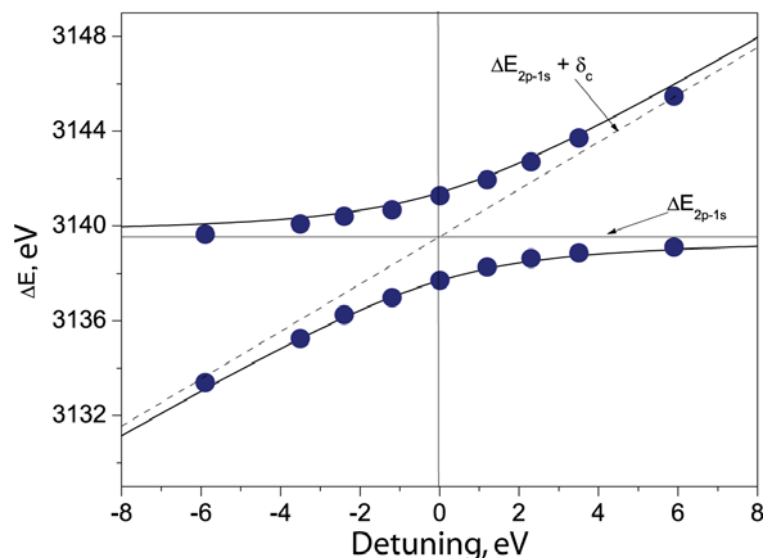
Autoionization in double RCE without channeling



Exp,: **Tokyo**
 Theory: **Moscow**,
 also strongly anisotropic angular distribution of the Auger electrons predicted



Autler-Townes effect in resonant coherent excitation of relativistic highly charged ions in crystals



PHYSICAL REVIEW

VOLUME 100, NUMBER 2

OCTOBER 15, 1955

Stark Effect in Rapidly Varying Fields*

S. H. AUTLER† AND C. H. TOWNES
Columbia University, New York, New York

(Received May 31, 1955)

A method is developed for calculating the effects of a strong oscillating field on two states of a quantum-mechanical system which are connected by a matrix element of the field. Explicit approximate solutions are obtained for a variety of special cases, and the results of numerical computations are given for others. The effect of an rf field on the $J=2 \rightarrow 1$ l -type doublet microwave absorption lines of OCS has been studied in particular both experimentally and theoretically. Each line was observed to split into two components when the frequency of the rf field was near 12.78 Mc or 38.28 Mc, which are the frequencies separating the $J=1$ and $J=2$ pairs of levels, respectively. By measuring the rf frequency, ν_1 , at which the microwave lines are split into two equally intense components, one may determine the separation between the energy levels. The measured value of ν_1 depends upon the intensity of the rf field and the form of this dependence has been calculated and found to be in good agreement with the experimental results.

Observation of the A-T doublet in current P&P measurements with lasers (an example)

PHYSICAL REVIEW A 78, 013802 (2008)

Observation of narrow Autler-Townes components in the resonant response of a dense atomic gas

Vladimir A. Sautenkov,^{1,2} Yuri V. Rostovtsev,¹ and Eric R. Eliel³

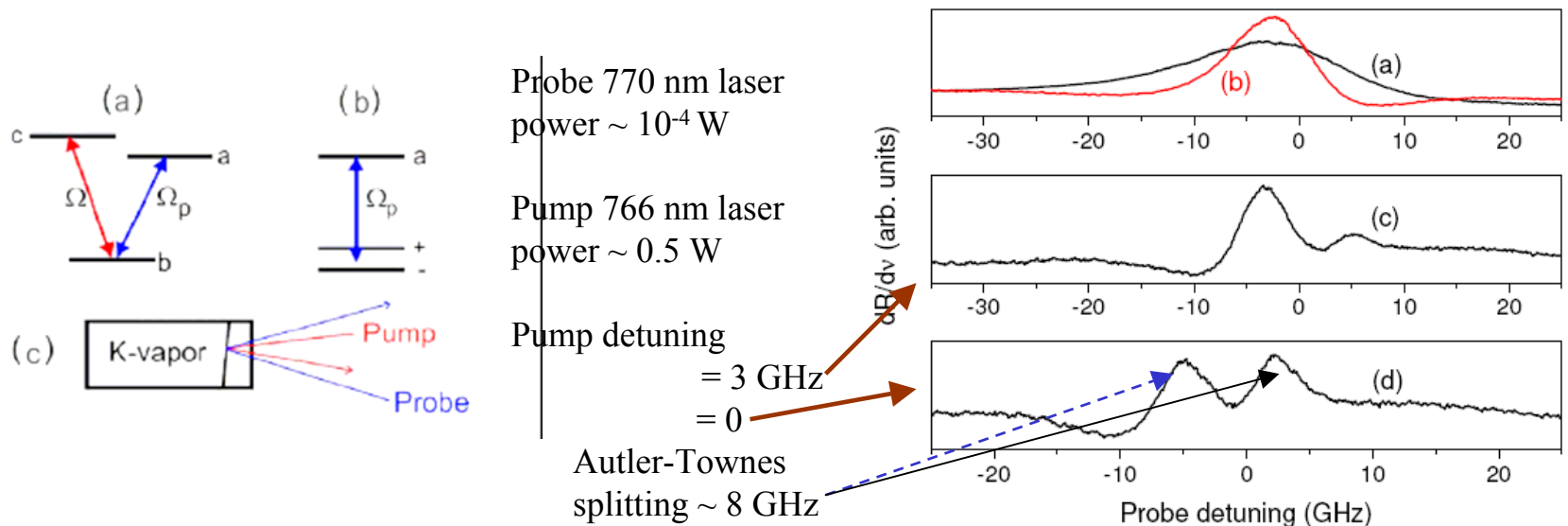
¹*Department of Physics and Institute of Quantum Studies, Texas A&M University, College Station, Texas 77843-4242, USA*

²*P. N. Lebedev Institute of Physics, 119991 Moscow, Russia*

³*Huygens Laboratory, Leiden University, P.O. Box 9504, 2300 RA Leiden, The Netherlands*

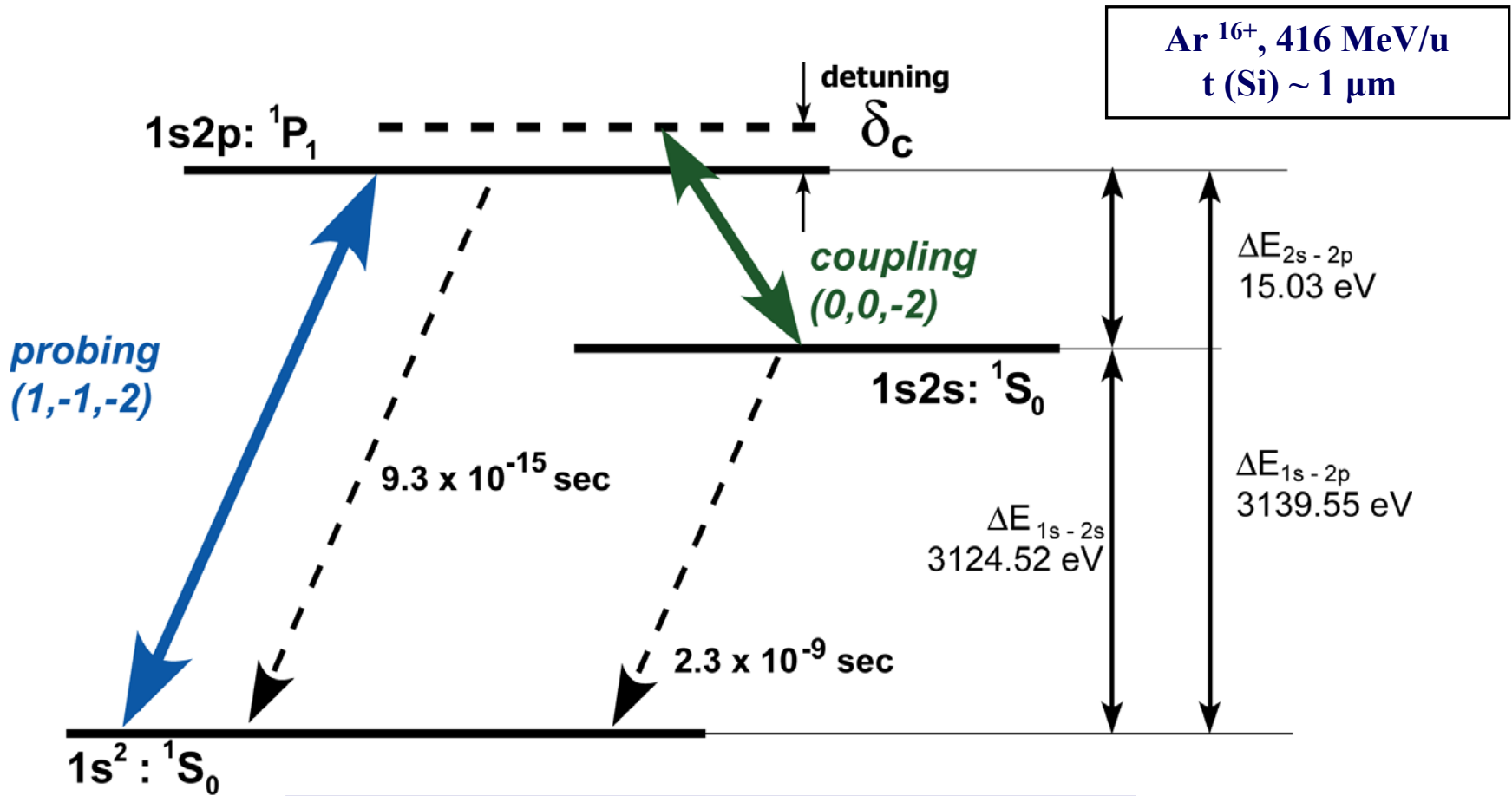
(Received 21 April 2008; published 1 July 2008)

We have experimentally studied the reflection of a weak probe beam from a dense atomic potassium vapor in the presence of a strong laser field tuned to the atomic resonance transition. We have observed an Autler-Townes doublet under hitherto unexplored conditions, namely, that the Rabi frequency induced by the strong laser field is much smaller than the self-broadened width of the resonance transition of the unexcited vapor. We attribute our observation to a reduction of the atomic decoherence by the strong drive field. We present a theoretical model of nonlinear processes in a dense atomic gas to explain the observed results.



Autler-Townes doublet at resonant coherent excitation (RCE) of relativistic ions in crystals without channeling

$$\omega_{k,l,m} = \frac{2\pi\hbar}{a} \gamma v (\sqrt{2}(k \cos\phi + m \sin\phi) \cos\theta + l \sin\theta)$$



Tuning in **coupling** и **probing** resonances – by target rotation

Both coupling and probing electric fields in the ion rest frame are strong:

$$\text{e.g.: } E_{(0,0,-2)}(1s2s:1S \leftrightarrow 1s2p:1P) \sim \mathbf{3.5 \cdot 10^9 \text{ V/cm}}$$

That corresponds to radiation energy flux of 15 eV - VUV laser of about $\mathbf{5 \cdot 10^{15} - 1.5 \cdot 10^{16} \text{ W/cm}^2}$. We calculated that a little lower energy flux of about $\mathbf{1.5 \cdot 10^{15} \text{ W/cm}^2}$ corresponds to 3140 eV – X-ray harmonic (0,1,2) of the probing field.

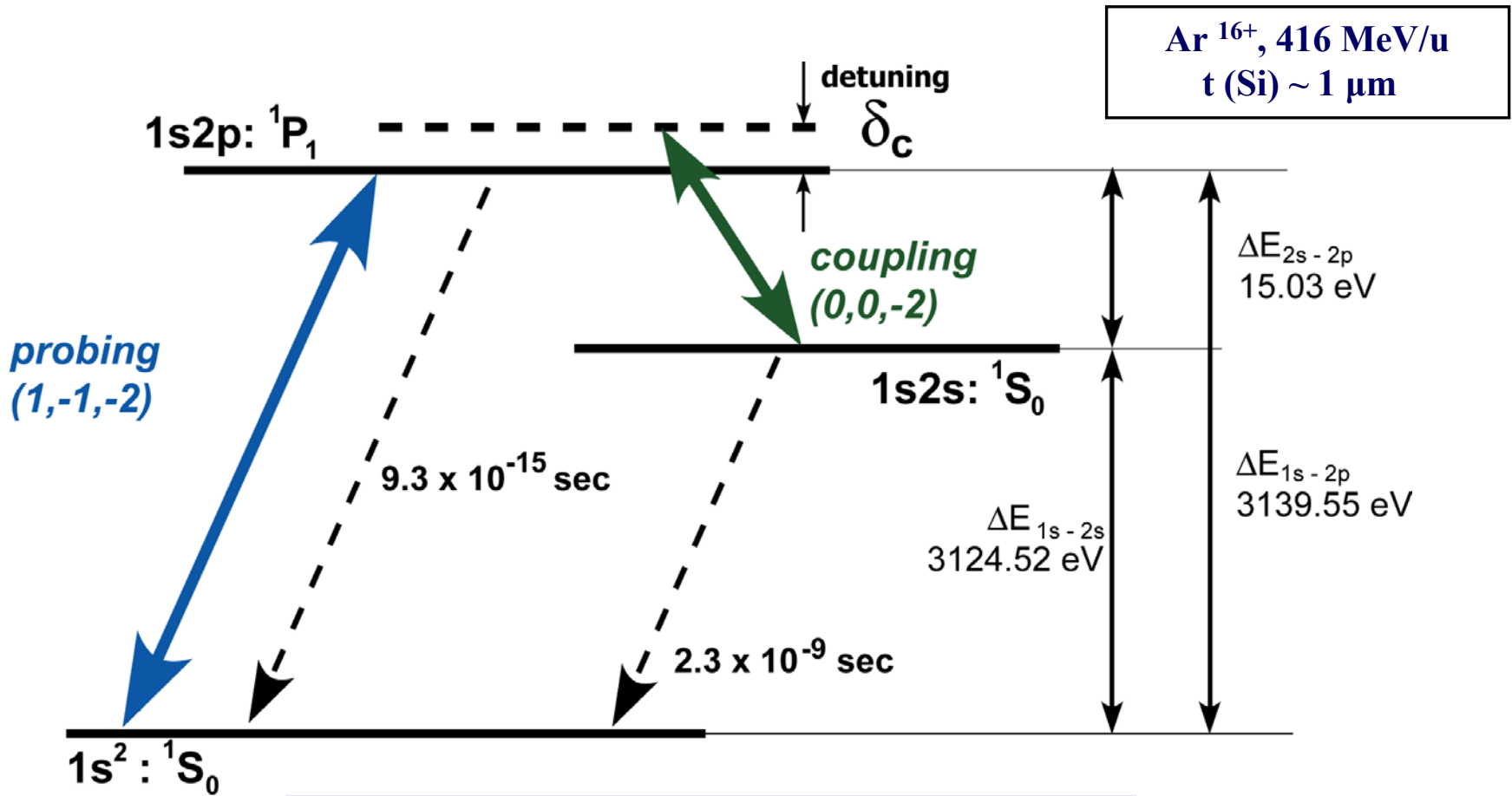
According to **Technical Design Report of the European XFEL** (pp. 264-274), the latter rate is near the lowest level of intensity of the flux for such suggested experiments on linear and non-linear processes as:

6.4.1. Small Quantum Systems

1. Inner shell ionization in atomic ions,
2. X-ray photons scattered at trapped ion crystals
3. Molecular dynamics following X-ray photoionization
4. Cluster experiments
5. Multiphoton studies in the X-ray spectral region
6. Dynamics of aligned small molecules and molecular wave packet dynamics
7. Time-resolved photo-fragmentation of small molecules

Autler-Townes doublet at resonant coherent excitation (RCE) of relativistic ions in crystals without channeling

$$\omega_{k,l,m} = \frac{2\pi\hbar}{a} \gamma v (\sqrt{2}(k \cos\phi + m \sin\phi) \cos\theta + l \sin\theta)$$



Tuning in **coupling** и **probing** resonances – by target rotation

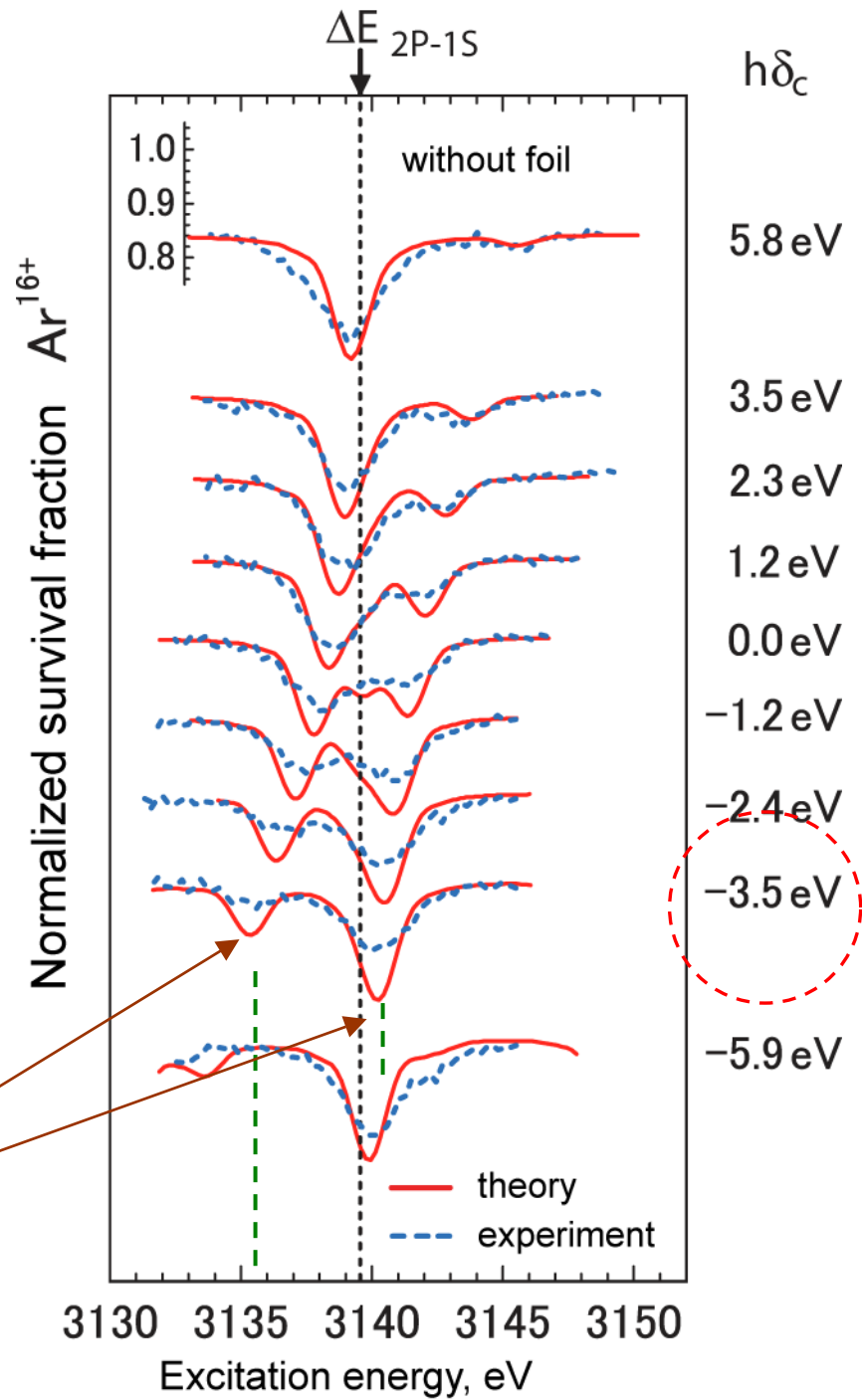
Survival fraction measurements

“Dressed atoms in flight through a periodic crystal field” –Y.Nakai, Y.Nakano, T.Azuma et al. - *Phys.Rev.Lett.* **101**, 113201 (2008)

“Kinetics of double resonant coherent excitation of relativistic multicharged ions in crystals beyond channeling conditions” – V.V.Balashov, A.A.Sokolik, A.V.Stysin - *JETP* **108** (2009) 1010

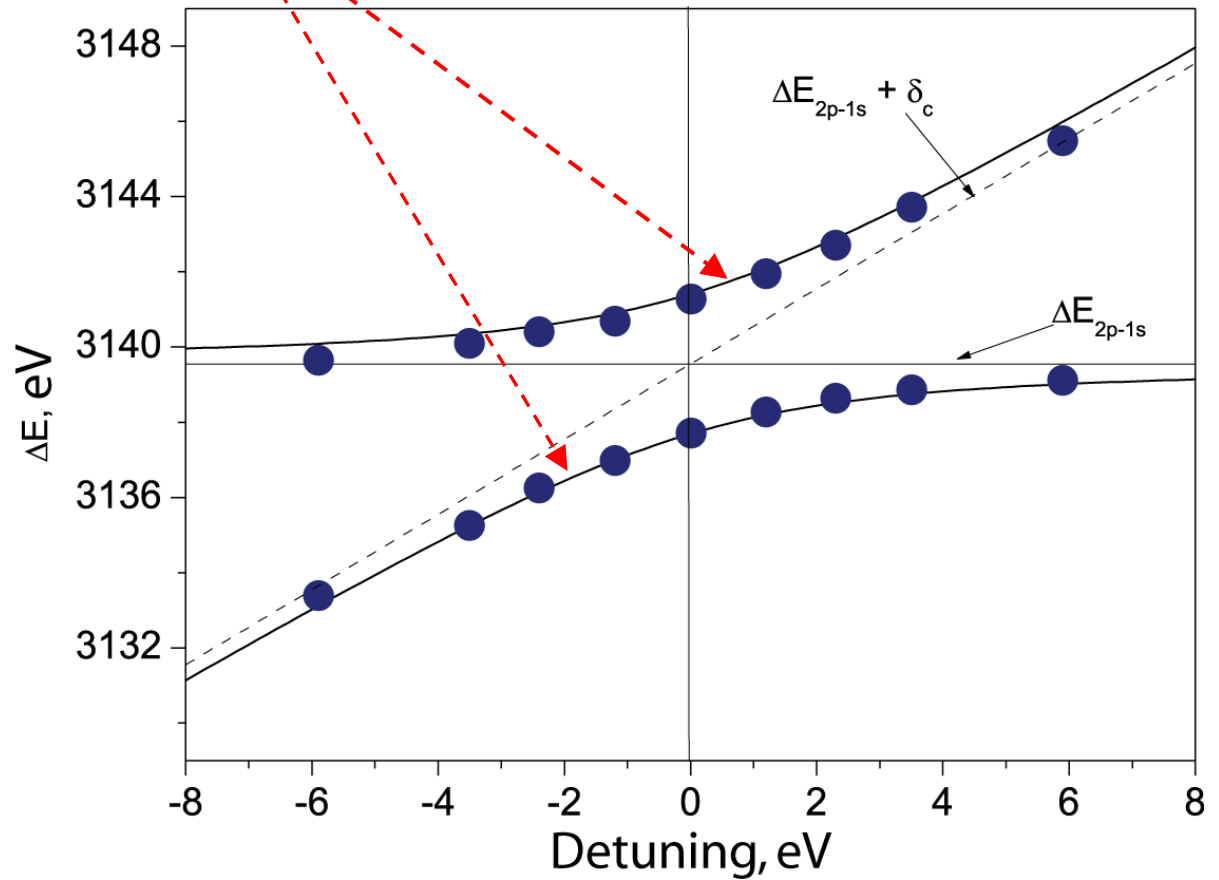
Red lines –calculation
with 5x5 density matrix in basis
 $1s^2: ^1S_0; 1s2s: ^1S_0; 1s2p: ^1P_1(M=0; \pm 1)$.

No fitting parameters.

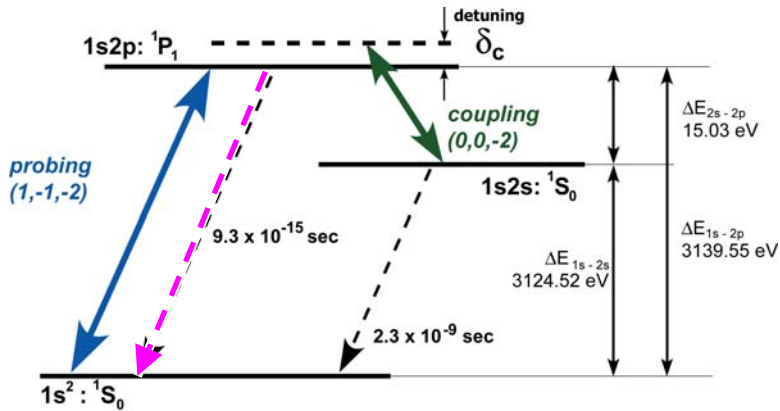


$$\Delta E_d^{(\pm)} = \Delta E_{2P-2S} + \frac{1}{2}[\hbar\delta_c \pm \sqrt{|\hbar\Omega_0|^2 + (\hbar\delta_c)^2}]$$

Ω_0 as a fitting parameter in the
 Autler-Townes formula =
 = **3.72 eV**;
 Ω_0 as calculated matrix element
 $\langle 1s2p: {}^1P_1 | V_{0,0,2} | 1s2s: {}^1S_0 \rangle$
 of the field
 = **3.55 eV**

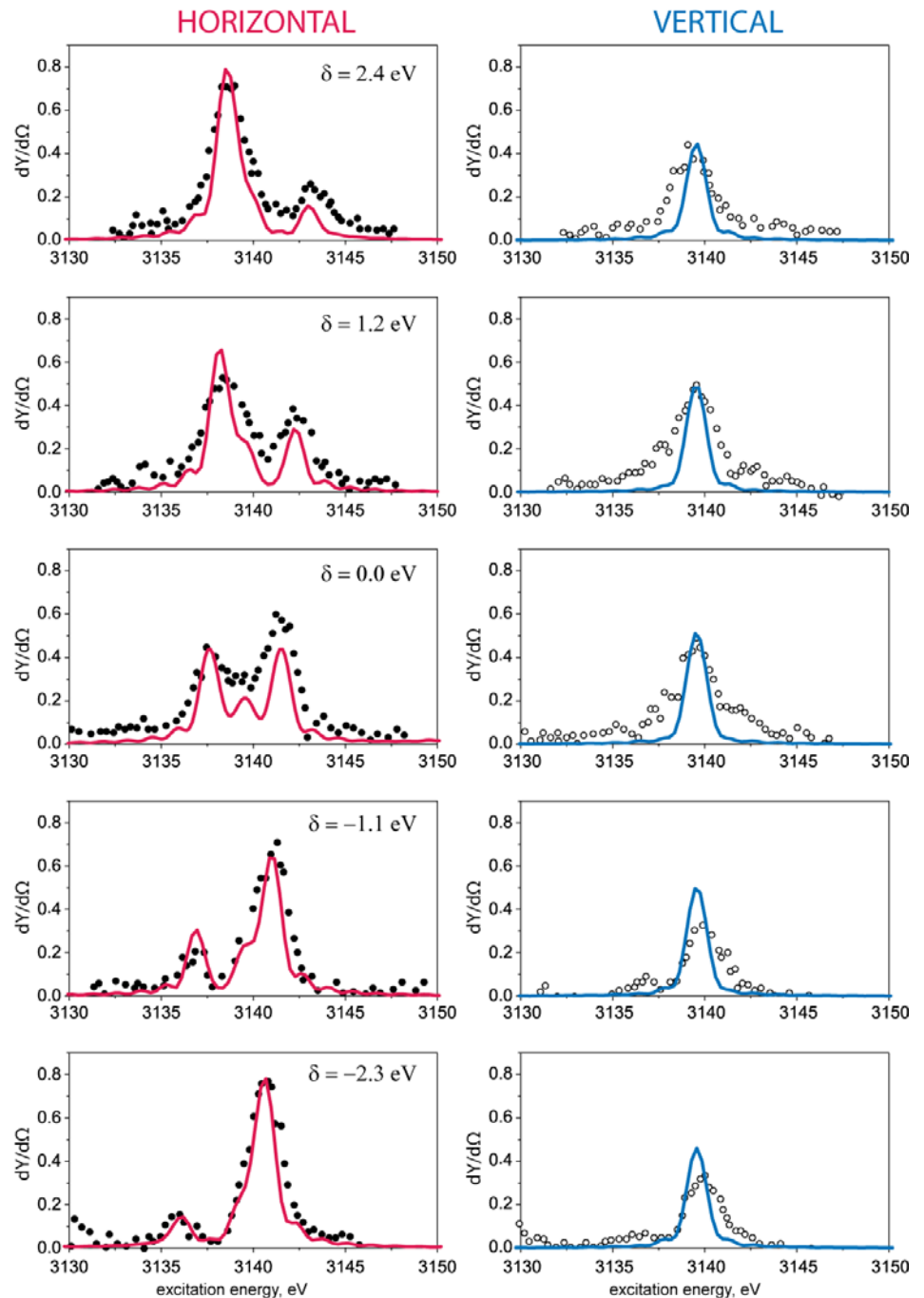


Autler-Townes doublet in characteristic X-ray radiation at double resonant coherent excitation



Drastic change in both experiment and calculation [JETP 108 (2009) 1010] in profile of the Autler-Townes doublet for X-ray photons detected in the (2,-2,0) plane direction [horizontal] and perpendicular to this plane [vertical] - clear demonstration of the potential of the Autler-Townes scheme in X-ray measurements to control polarization characteristics of double excitation of highly charged ions.

Here - indication to “fine structure” magnetic quantum number splitting of the Autler-Townes doublet $1s2s: ^1S_0 \leftrightarrow 1s2p: ^1P_{M=0; \pm 1}$.



Conclusion

The insightful prediction on resonant coherent excitation of fast ions in crystals made 45 years ago by Okorokov opened a way to wide experimental and theoretical investigations of this nice phenomenon. Basic parameters of currently studied RCE processes with relativistic highly charged ions (produced photon energy, radiation energy flux in the ion rest frame) look close to those usually related to XFELs. Also, one cannot ignore a unique feature of RCE as a tunable source of polarized X-ray radiation. True, RCE will never compete with lasers in whole. But wide experience gained in experimental and theoretical RCE studies, especially concerning polarization aspects of dynamics of various multi-photon processes in keV energy region, will be a good support among others for future XFEL experiments.

Deep thanks

to my RCE co-authors and co-workers

I.Bodrenko,
A.Sokolik,
A.Stysin,
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Angular Correlation of the Cascade Photons in the Course of Dielectronic Recombination of Channeled Ions

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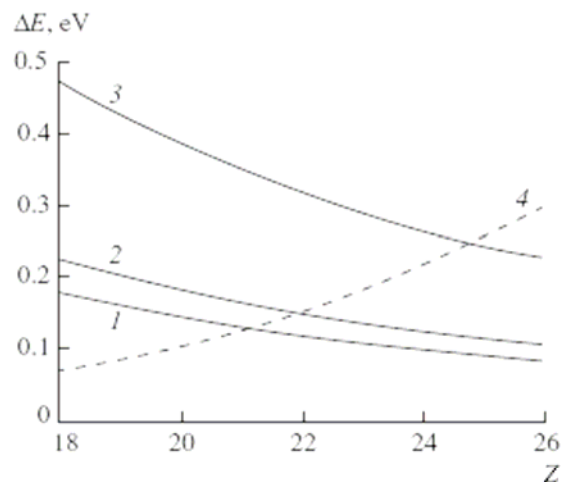


Fig. 1. Splitting (8) of the $1s2p : ^1P_1$ level in an ion from argon Ar^{16+} to iron Fe^{24+} in the plane $(2\bar{2}0)$ channel of the silicon crystal: (1) at the center of the channel and on departure from the center by (2) 0.3 and (3) 0.6 channel half-width; (4) radiation width Γ of this level.