

Relativistic Electron Beam Dynamics in Crystals
and Related Electrodynamical Processes



Calculation of the dechanneling length of electrons in Si crystal using 3D binary collision model



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Model equations

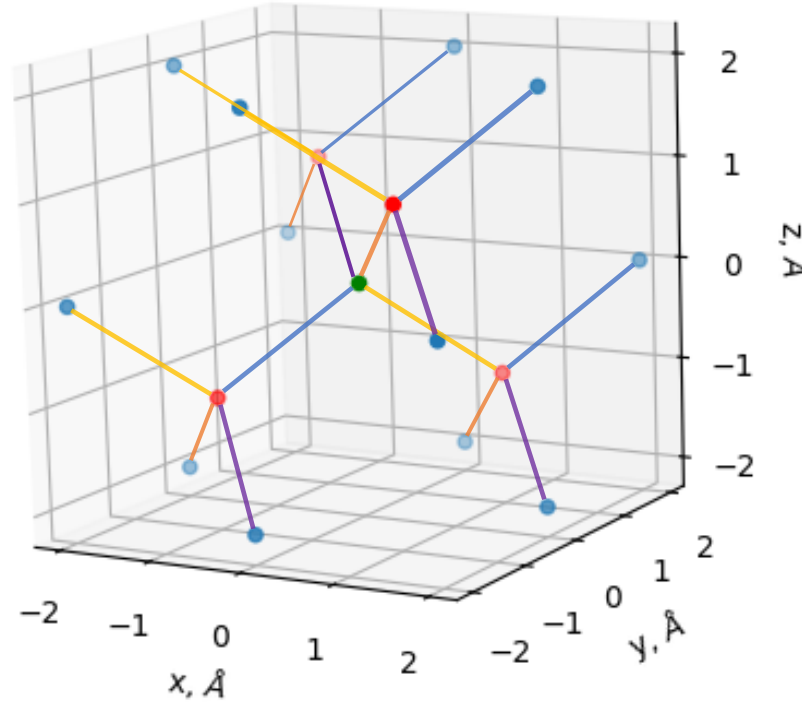
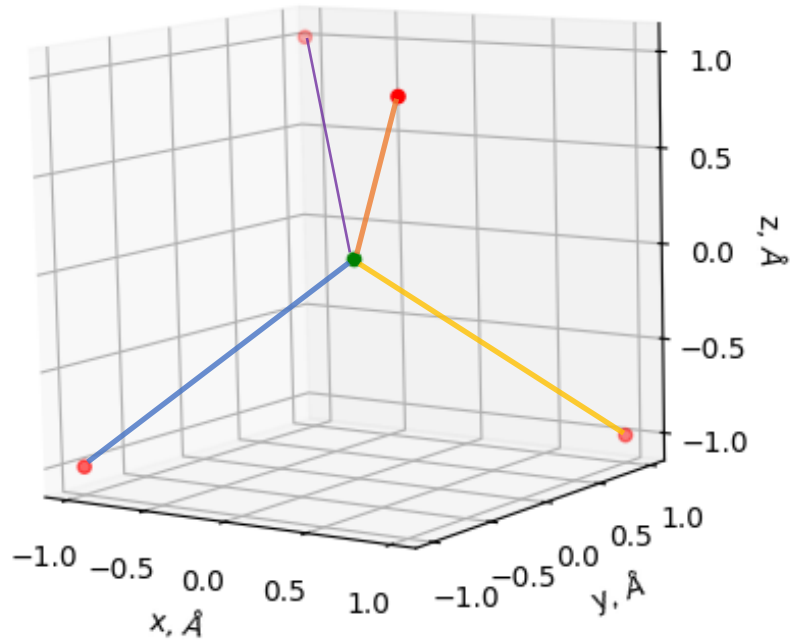
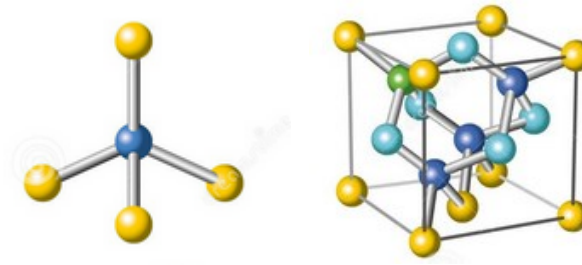
$$\left\{ \begin{array}{l} \frac{d\mathbf{p}}{dt} = -q\nabla_{\mathbf{r}}U(r) \\ \frac{d\mathbf{r}}{dt} = \mathbf{v} \end{array} \right. \quad U_M(r) = \frac{Z_2 e}{4\pi\epsilon_0 \cdot r} \chi(r); \chi(r) = \sum_{j=1}^3 \alpha_j \exp\left[-\frac{\beta_j r}{R_S}\right]$$

$$\check{t} = ct; \quad \check{p}_x = \frac{p_x}{mc}; \quad \check{p}_y = \frac{p_y}{mc}; \quad \check{p}_z = \frac{p_z}{mc}; \quad \mu_i \equiv \frac{Z_1 Z_2 \alpha \hbar c \alpha_i}{mc^2}; \quad B_i \equiv \frac{\beta_i}{R_S}$$

$$P_M(r) = qU_M(r) = \frac{1}{r} \sum_{j=1}^3 \mu_j \exp[-B_j r]; \quad \nabla_{\mathbf{r}} P_M(r) = -\mathbf{r} P'_M(r);$$

$$P'_M(r) = \frac{1}{r^2} \sum_{i=1}^3 \left(B_i + \frac{1}{r} \right) \mu_i \exp[-r B_i]; \quad \left\{ \begin{array}{l} \frac{d\check{\mathbf{p}}}{d\check{t}} = \mathbf{r} P'_M(r) \\ \frac{d\mathbf{r}}{d\check{t}} = \frac{\check{\mathbf{p}}}{\gamma} \end{array} \right.$$

Multiple atoms' field



$$P'(r) = \sum_i P'_M(|\mathbf{r} - \mathbf{r}_i|)$$

$$\begin{cases} \frac{d\check{\mathbf{p}}}{d\check{t}} = \mathbf{r}P'(r) \\ \frac{d\mathbf{r}}{d\check{t}} = \frac{\check{\mathbf{p}}}{\gamma} \end{cases}$$

Adding thermal vibrations $\Delta\mathbf{r}_i$: $f(\Delta\mathbf{r}_{i(x,y,z)}) = \frac{1}{\sqrt{2\pi u_T^2}} \exp\left[-\frac{\Delta r_{i(x,y,z)}^2}{2u_T^2}\right]$

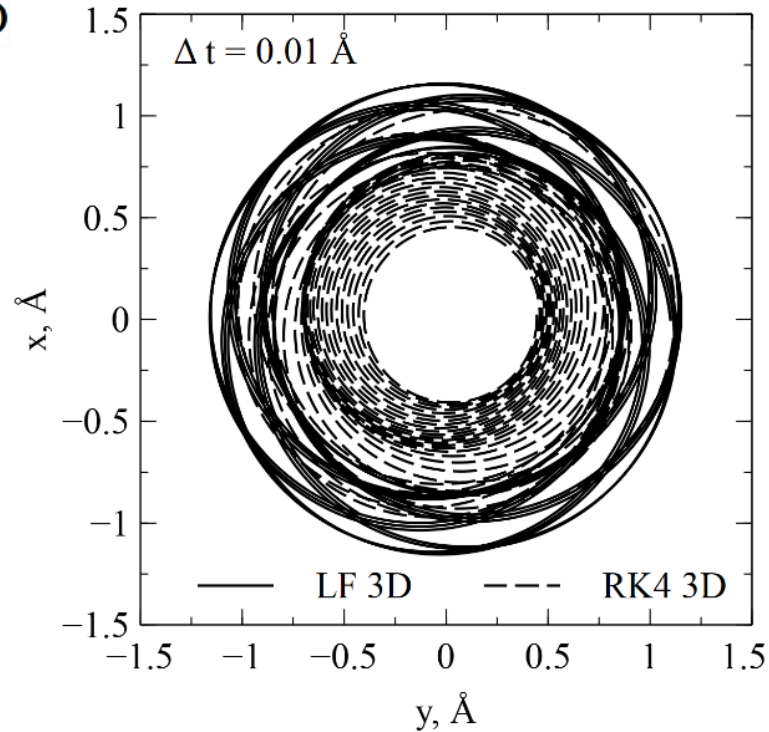
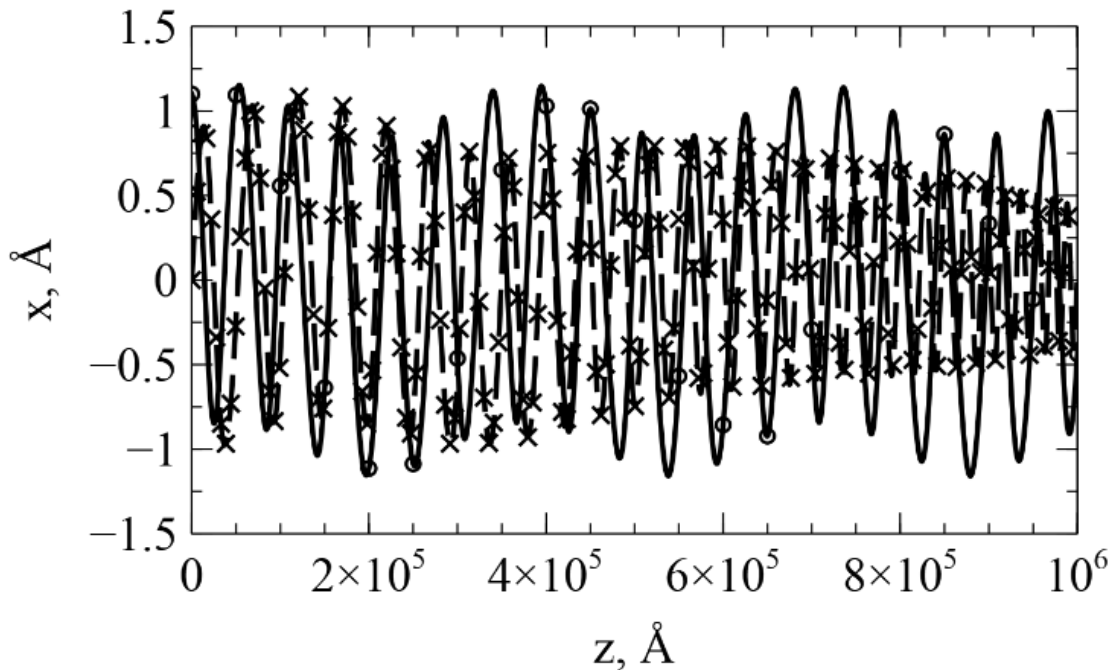
Comparison of the RK4 and leapfrog solvers

for calculations without thermal vibrations, along a chain of atoms

RK4 – Runge-Kutta integrator of the fourth order, error is on the order of $O(h^4)$

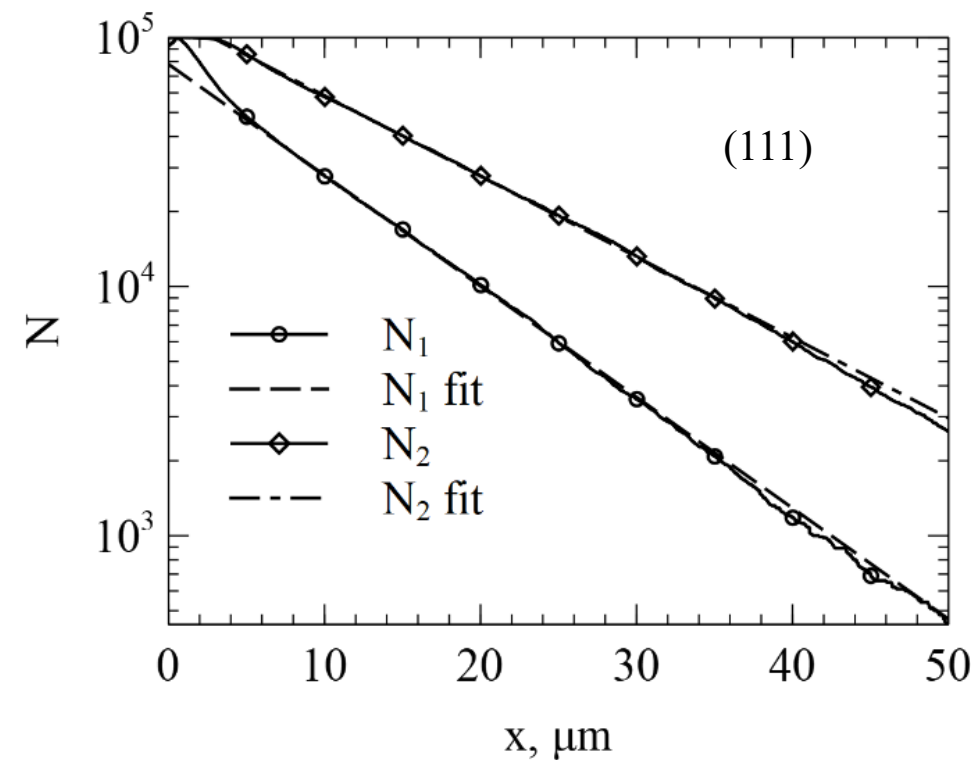
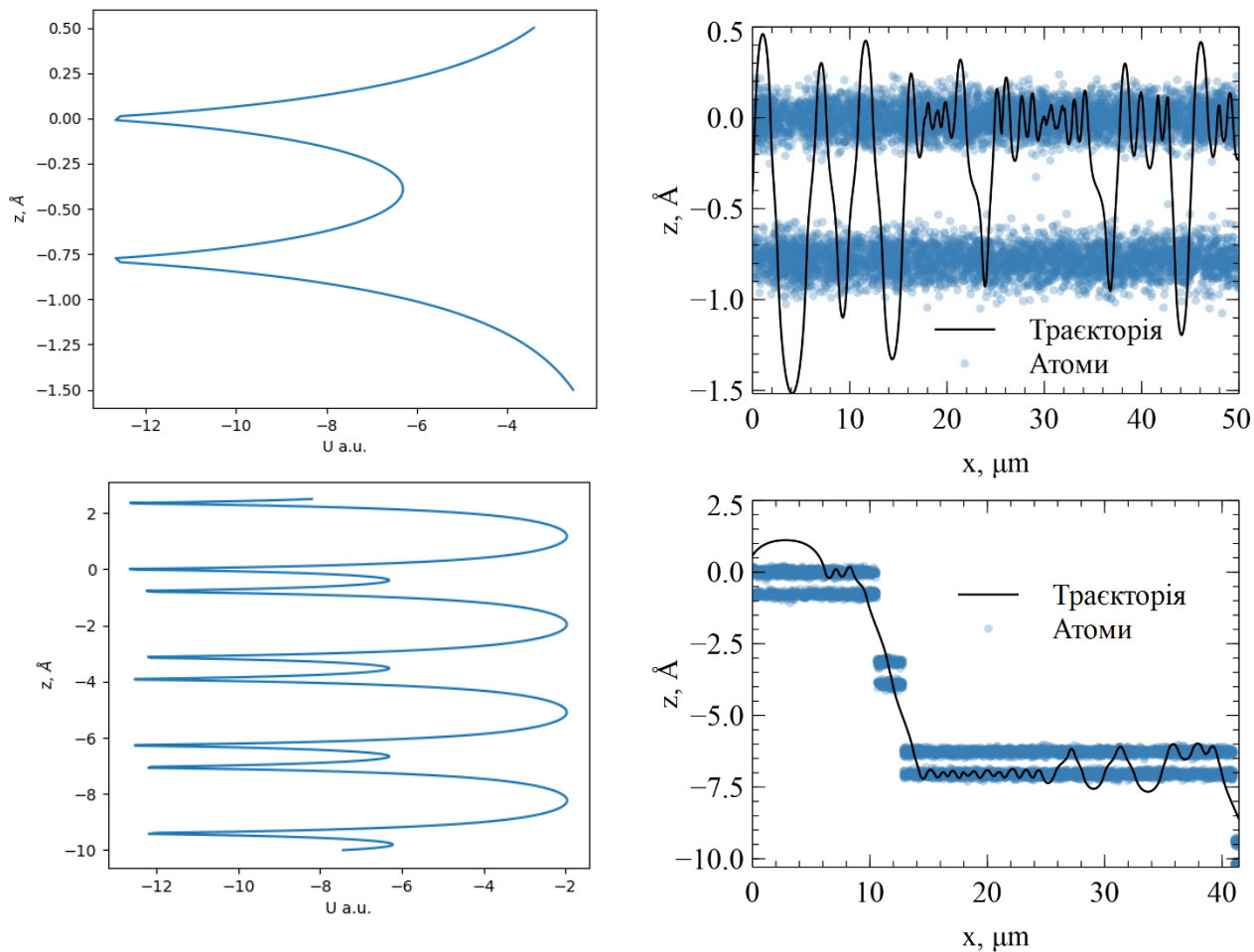
LF – leapfrog integrator, error is on the order of $O(h^2)$

$\Delta t = 0.01 \text{ \AA}$ —○— LF 3D —×— RK4 3D



leapfrog integrator:
 $\mathbf{a}_i = \mathbf{r}_i P'_M(\mathbf{r}_i)$
 $\mathbf{v}_{i+1/2} = \mathbf{v}_i + \mathbf{a}_i \frac{\Delta t}{2}$
 $\mathbf{r}_{i+1} = \mathbf{r}_i + \mathbf{v}_{i+1/2} \Delta t$
 $\mathbf{v}_{i+1} = \mathbf{v}_{i+1/2} + \mathbf{a}_{i+1} \frac{\Delta t}{2}$

Planar channeling in the (111) plane of Si crystal, e^- , $E = 885$ MeV



Without rechanneling

$$N_1 \sim \exp[-x/9.75 \mu\text{m}] ; (11.01 \mu\text{m}/\text{GeV})$$

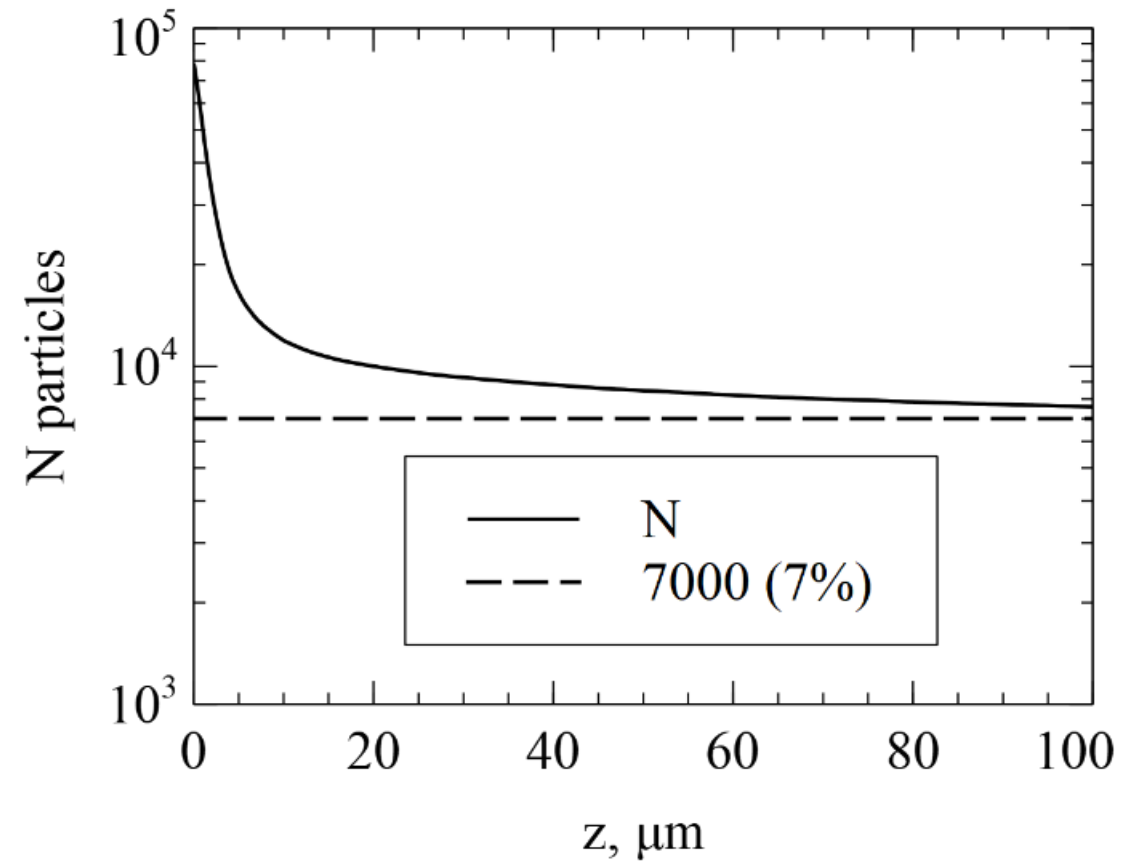
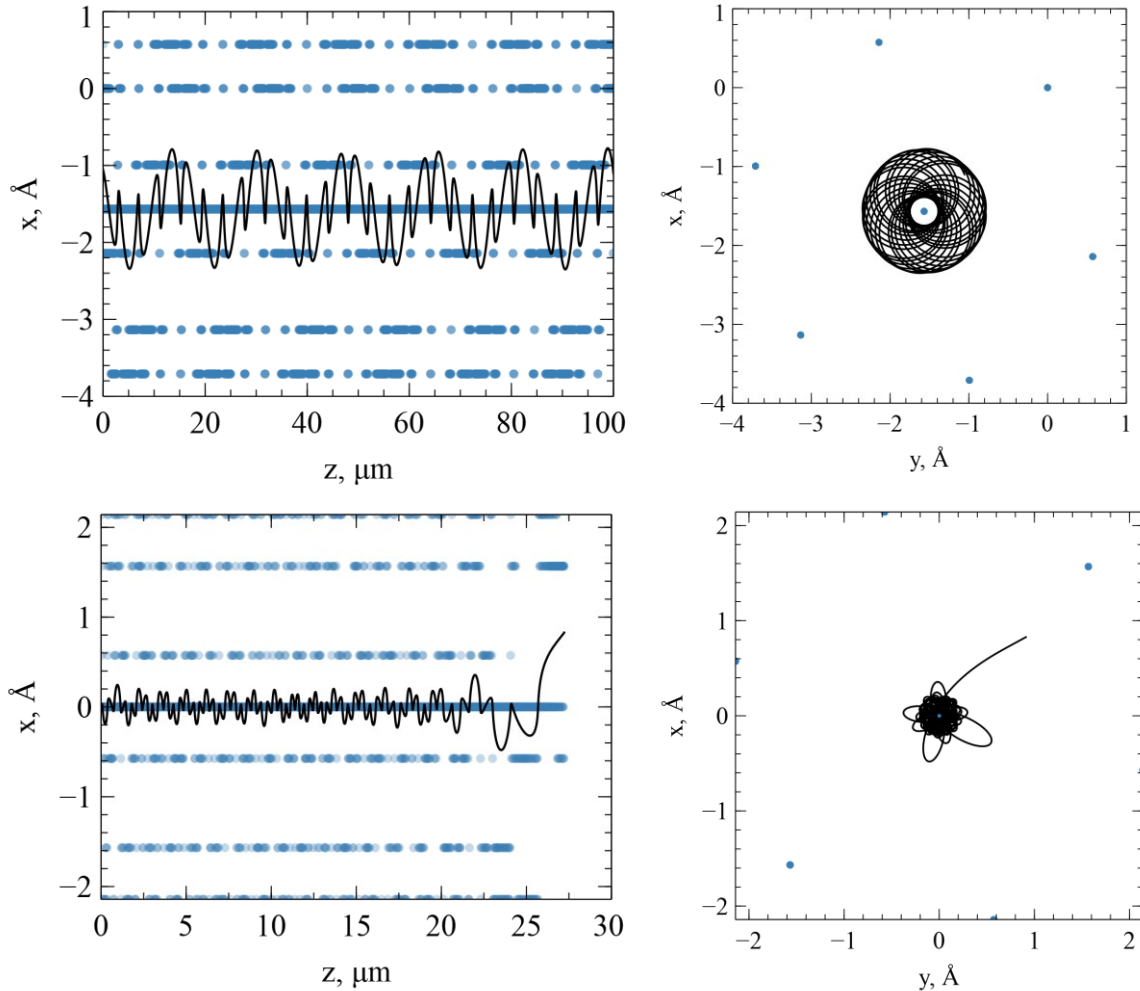
With two rechannels

$$N_2 \sim \exp[-x/13.41 \mu\text{m}] ; (15.16 \mu\text{m}/\text{GeV})$$

U. Wienands et.al. Channeling, volume reflection, and volume capture study of electrons in a bent silicon crystal. PHYSICAL REVIEW ACCELERATORS AND BEAMS. 19, 071001 (2016). $L_D \approx 15.3 \mu\text{m}/\text{GeV}$

Axial channeling along $\langle 111 \rangle$ axis of Si crystal, e^- , $E = 1$ GeV

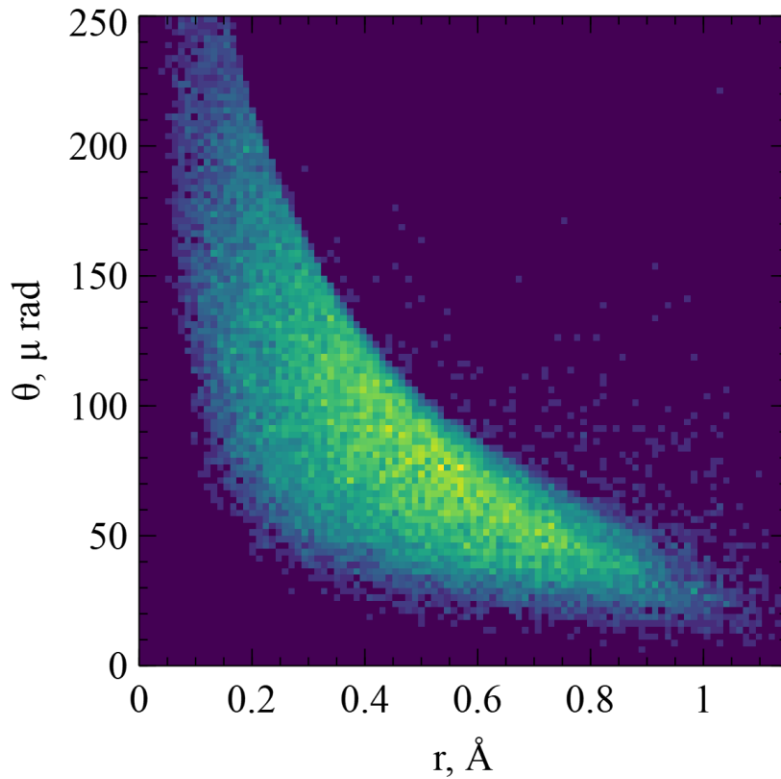
without thermal vibrations



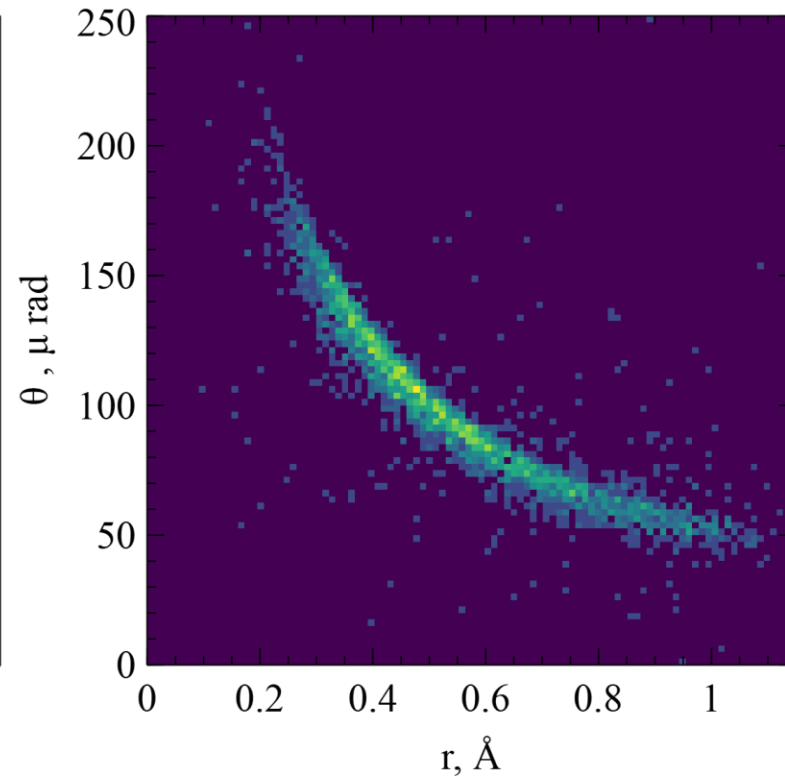
Distribution of particles that remain in the channeling regime

Distribution of particles (brighter zones – more particles), that remain in the channel after passing 20 μm of crystal

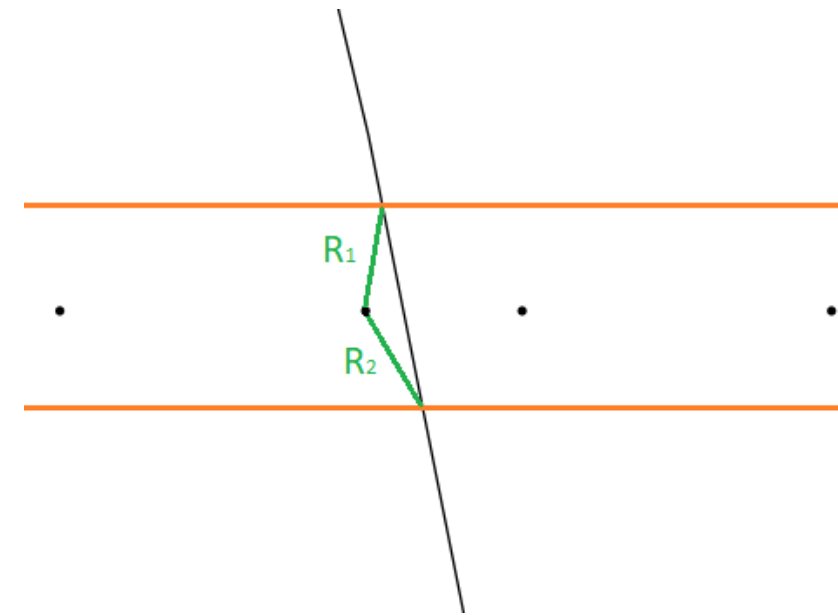
without thermal vibrations



with thermal vibrations



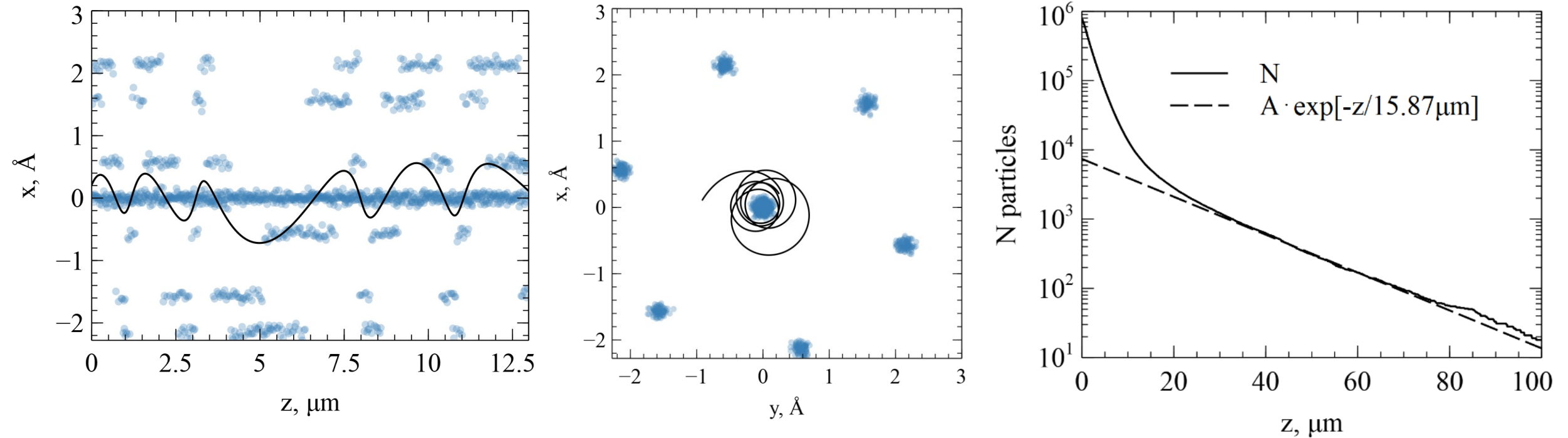
dechanneling on individual atoms in binary collision model



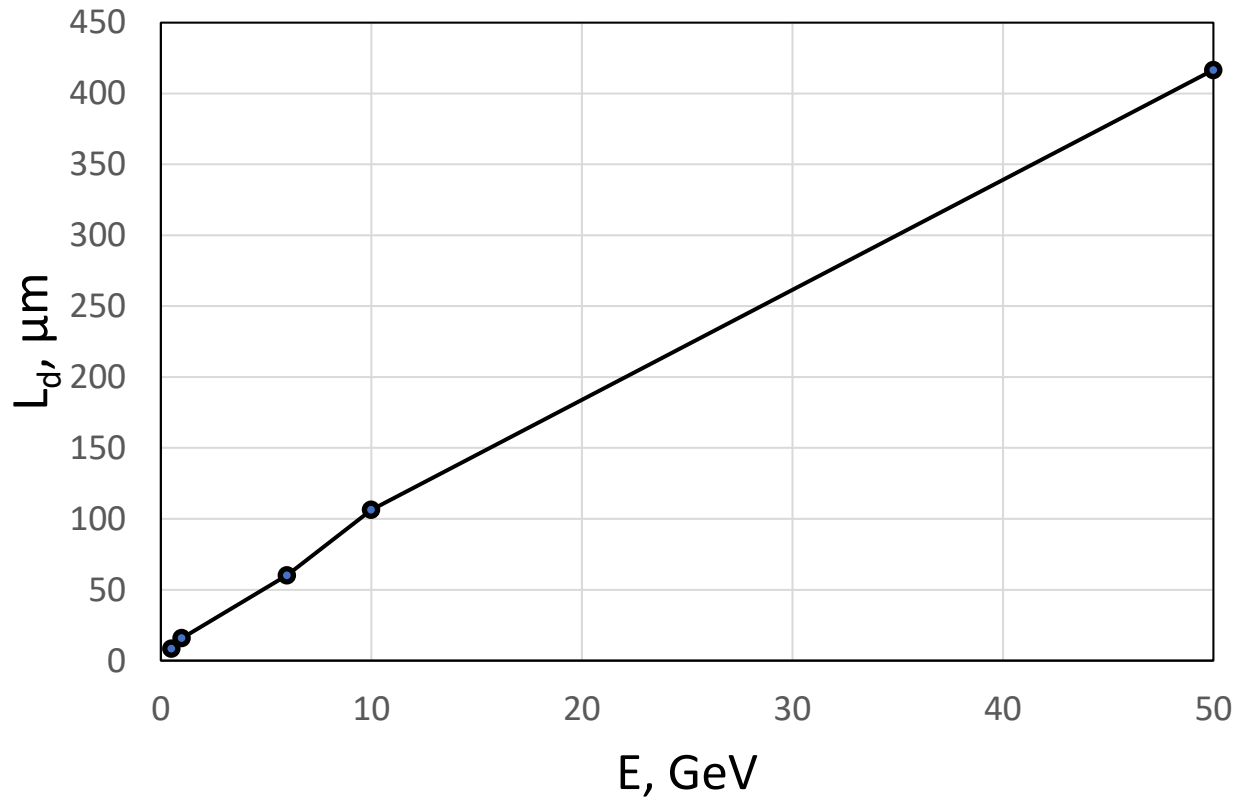
quantum mechanics needs to be applied!

Axial channeling along $\langle 111 \rangle$ axis of Si crystal, e^- , $E = 1$ GeV

with thermal vibrations



Dechanneling length for different energies



E, GeV	L_D , μm	L_D/E , $\mu\text{m}/\text{GeV}$
0.1	1.73	17.32
0.5	8.50	17.00
1.0	15.87	15.87
6.0	60.24	10.04
10.0	106.38	10.64
50.0	416.67	8.33

Thank you!

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Choosing optimal calculation step

$$y(t_0 + h) = y(t_0) + hy'(t_0) + \frac{1}{2}h^2y''(t_0) + O(h^3)$$

$$y'(t_0) = \frac{y(t_0 + h) - y(t_0)}{h} - \frac{1}{2}hy''(t_0) + O(h^2)$$

$$\Delta\check{t} = (1 - \exp[-r/1 \text{ \AA}]) \cdot (\Delta\check{t}_{\max} - \Delta\check{t}_{\min}) + \Delta\check{t}_{\min}$$

