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A sub-atomic microscope, superfocusing in channeling and close encounter atomic and nuclear reactions

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Abstract. A highly collimated beam of protons (≈1 MeV) entering the channel of a monocrystal film forms at a certain depth an extremely sharp (<0.005 nm) and relatively long (some monolayers of the crystal) focusing area where the increase of the flux density can reach thousand times. Impinging atoms in this focusing area can undergo nuclear or atomic reactions with proper foreign dopants which disappear if the crystal is tilted from this position by only 10^{-3} radians. This effect can be called channeling superfocusing, in contrast to the ordinary fluxpeaking where the increase of flux density reaches only few times. Results are predicted by quantum mechanical model calculations and confirmed by channeling Monte Carlo simulations accounting for several properties of the real lattice.

PACS. 61.85.+p Channeling phenomena (blocking, energy loss, etc.) – 34.20.-b Interatomic and intermolecular potentials and forces, potential energy surfaces for collisions – 34.70.+e Charge transfer – 34.80.-i Electron scattering

A somewhat provocative title is chosen to attract the attention to these problems. Considered together they may lead to some promising directions of research. The present development in microphysics and in microtechnology allows us to construct experimental devices on atomic scale. Channels in a monocrystal are one of such "devices". Combining macroscopic length with microscopic width allows one to build a bridge between both regions.

Let us consider a thin monocrystal film with hundreds of monolayers and with channels perpendicular to the surface. All of them transmit charged particles (e.g. energetic protons of ≈1 Mev) with small energy loss and small momentum transfer across the whole film. The mean effective potential of the channel can be calculated easily and the deflection of the fast particle within the channel can be found. In many cases the potential of the central part of the averaged channel is cylindrically symmetric and harmonic to a good approximation and it creates isochronic oscillations of the ions in the plane normal to the direction of the channel. It is possible to adjust the strength of the central 2-dimensional channel paraxial potential, the velocity of the incident particles and their masses, so that they will be focused together into a sharp and relatively long focus (some tens of monolayers) on the rear side of the film and on the axis of the channel. The radius of this focus can in principle be very small, less than 10^{-2} nm. This looks fantastically small and is even less than the thermal vibrational amplitude of a single atom in the lattice. So we have a needle-like focusing area where the flux density of particles increases more than hundreds times relative to the initial one outside of the lattice! Such an unprecedented sharpness of the focusing peak allows us to call this effect the super-focusing. Previously there were experiments and theoretical papers investigating the distribution of momenta of particles across the channel resulting in rainbow like distributions [1] and peaked structures [2,3]. Also planar channeling, resulting in a depth dependent line-focusing, is calculated theoretically by several authors and experimentally used to localize impurities by RBS with a resolution of the thermal vibrational length of the host single crystal [4–6]. However, axial peak-focusing (super-focusing) was not really considered in these investigations.

The above mentioned superfocusing needs a very good collimation of the incident particles. The beam divergence has to be better than 2×10^{-4} radians. In this case many of the incoming trajectories do not leave the paraxial harmonic region before focusing after a quarter of the transverse oscillation period $T/4$ occurs. If this focusing occurs near the rear side of the film, we can impinge the ions on to a different sort of foreign atoms in the channels of the film near the rear surface and register their collisions by e.g. induced nuclear reactions [7] or increase of atomic X-ray fluorescence yield [8] when the positions of the foreign atoms coincide with the focus. Tilting the film by such a small angle as 10^{-4} radians will reduce the collision probability

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and the observed reaction yield will sharply decrease. One should keep in mind that only the paraxial part of the incident beam is focused and this is presumed to be in the order of ten percent of the whole beam (however, the other major part of the beam contributes only weakly to the enhanced collision probability). This allows one to find the positions of impinging atoms relative to the channel and to analyse the sharpness of the focus. Further on, this arrangement can be seen as a two-dimensional periodical array of nuclear microscopes for the target atoms with the periodicity of the focusing lattice.

Eventually one can even improve the film detection efficiency further by adding to it epitaxially some number of layers with foreign atoms, with the interstitial position of these dopants just across the centers of the channels. The focused beam will coincide with these rows of atoms and the rate of reactions will increase further.

Another, experimentally more fastidious possibility occurs if we impinge the film from both sides by two different sorts of beams of light nuclei chosen to have a large cross section for a low-energy nuclear reaction (e.g. a deuterium deuterium reaction [9]), so that both beams are exactly opposite to each other. The particles will then be focused in the center of the channels and near the middle of the film where the lattice is more regular than at the surface. Because both focused regions are elongated along the channel axis the overlapping could be maximalized considerably. Periodical repetition of the focusing of both beams by $T/2$ oscillations will make the mutual reaction volume several times larger. Such a merging of the focuses within the channel in case of opposite beams makes the size of the focus and the size of the target almost equal which is the most favorable case.

Probably there exist other possible improvements of dynamic micro-regulations for beams of particles. Such dynamical manipulations with the system of particles using Liouville's theorem and transforming high concentration in the momentum space (collinearity) into the concentration in the coordinate space (focusing), which is demonstrated here, shows evidently how these theoretical facts can help to understand the possibilities in interaction of beams and solids, including, as a distant perspective the macroscopical release of the nuclear energy.

1 Quantum mechanical model

These preliminary considerations can be supported by the solution of an exactly solvable quantum mechanical model approximating the channel averaged potential (independent of the channel direction z) by a 2-dimensional oscillator potential proportional to $(x^2+y^2)/2$ for the transverse direction. For the energy of the beam considered and to separate the coordinates we can treat the z motion along the channel classically and replace z by the time t setting the velocity equal to unity. Then the Schrödinger equation for the x part of the potential will be:

$$\left(-\frac{1}{2}\frac{\partial^2}{\partial x^2}+\frac{1}{2}x^2\right)\,\psi(x,t)=i\,\frac{\partial\,\psi(x,t)}{\partial\,t}$$

with a given starting wave function:

$$\psi(x,0)=\pi^{-1/4}\,R_s^{-1/2}\,\exp\left(-x^2/(2R_s^2)\right)$$

where R_s is the initial radius of the beam area within the channel where our harmonic approximation of the potential holds. The value of R_s could be one half to one third of the channel radius under consideration. This non stationary Schrödinger equation can be solved using a Green functions approach for the harmonic oscillator [10].

$$G(x',\,x,\,t)=\pi^{-\frac{1}{4}}(2\,\pi\,\sin(t))^{-\frac{1}{2}}\cdot \exp[(i/2)\,(x^2+x'^2)\cot(t)-i\,(x\,x'/\sin(t)-\pi/4)].$$

From the general formula:

$$\psi(x,\,t)=\int G(x',\,x,\,t)\,\psi(x',\,0)\,dx'$$

an important property of this oscillator Green function can be exploited: it depends exponentially on x and x' and is purely quadratic in the exponent. Therefore the integral can be calculated explicitly for any initial exponential wave function depending quadratically and linearly on x'. Performing these calculations we get:

$$|\psi\,(x,y,t)|^2=N^2(t)\exp\left[-\frac{(x+p_x\,\sin(t))^2+y^2}{(R_s\cos(t))^2+(R_{min}\sin(t))^2}\right].$$

Here we multiplied $\psi(x,\,t)$ by the corresponding $\psi(y,\,t)$ but without the p_x term. This p_x term describes a possible tilting of the beam axis relative to the x axis of the channel leading to the appearance of the additional factor $\exp(i\,p_x\,x)$ in the starting $\psi(x,\,0)$.

The crucial parameter defining the rate of focusing is $\mu = R_s/R_0$ the relation between R_s the oscillator like size of the average potential and R_0 the size of the ground state transverse wave function. The product $R_s \cdot R_{min} = R_0^2$, where $R_0^2 = 1$ in our units and $R_0^2 = \hbar/M\,\omega$ in arbitrary units. The compression in the focusing area is $R_s^2/R_{min}^2 = \mu^4$. In case of hydrogen ions and a silicon monocrystal μ can reach 6, the compression more than 1000!

From Figure 1 can be seen that all properties discussed before are present here: The above solution is "breathing" between R_s and R_{min} with a period $T = \pi/2$. The focusing point appears in coordinate space at the time $\pi/2$, $3\,\pi/2$, $5\,\pi/2$, ... in the points $x = p_x$, $x = -p_x$, $x = p_x$.

2 Computer experiment

These considerations presented here are supported by Channeling Monte Carlo computer experiments [11] performed by one of us (J.D.M.) for up to 2 MeV protons impinging onto the $\langle 100\rangle$ direction of silicon. The angular divergence of the ions is chosen ≤ 0.01 (1.75×10^{-4} rad). Every step of our simulation includes the ion steering induced by the thermally vibrating lattice atoms up to a

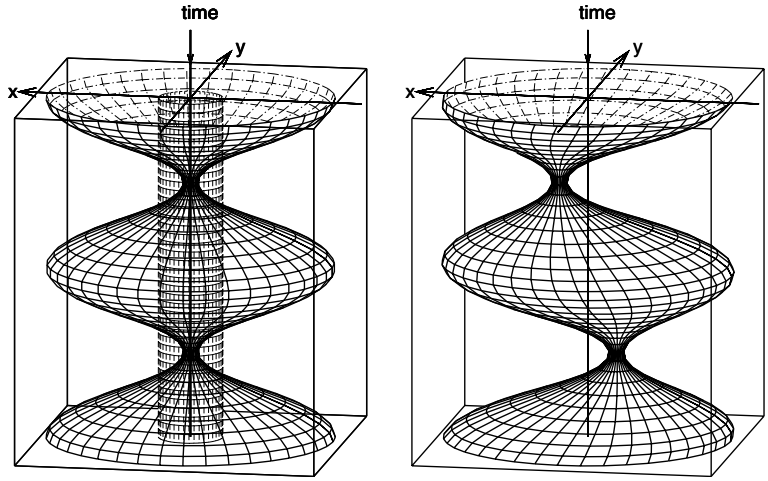

Fig. 1. Surface of the area where the density $|\psi(x, y, t)|^2$ drops to $1/\sqrt{e}$. The particle enters from the top. On the left hand side p_x is zero (no tilting of the channel). The surface is "breathing" as a function of time (depth). The equilibrium solution of the Schödinger equation for $R_0 = R_s = R_{min}$ is underlayed. On the right hand side a tilting of the channel in x direction ($p_x > 0$) for the starting wave function shows the oscillation of the focus point around the center of the channel as a function of time.

distance of 0.6 nm from the moving ion. Each atoms vibration around its lattice equilibrium position is picked for all tree spatial axes from the elements of an ensemble of Gaussian distributed numbers with mean zero and a width of the thermal vibrational amplitude $\rho_{th} = 0.0078$ nm. Electronic and nuclear scattering as well as electronic [12] and nuclear energy loss of the ions in the lattice are also included. Charge transfer effects of the ions are taken into account. Different model potentials (statistical models: Moliere and Universal potential [13]; solid state models: Hartree Fock [14]) were probed for the ion-lattice atom interaction. Here we shall point out only some results of our simulations in relation to the topics of this paper.

2.1 Comments to the pictures

The main property of the harmonic oscillator: the repeated focusing in the coordinate and the momentum plane is evident from Figure 2. It is known that the ideal lens transforms the image plain into its Fourier transform. This property transforms the initial broad Gaussian wave function (low flux density) into an extremely narrow function at the focus. This "breathing" property of the beam within the channel was expected (see Fig. 1) and is proven by our computer experiments. The focusing repeats with increasing depth into the crystal with the period $T/2$ after the first focusing at the depth $T/4$ (in Fig. 2 at 35.0 nm). The sharpness and height decrease gradually depending on the angular divergence of the impinging ions and the scattering and energy loss processes of the ions. The repeated focusing is the direct evidence for the synchronous beam oscillations.

The focusing of the beam is extraordinary sharp in a plane perpendicular to the motion of the ions (Fig. 3). One can see that the peak is even sharpening at the top, which means that the sharpness (FWHM) is much smaller than 2 times $\rho_{th} = 0.0078$ nm, the thermal vibrational amplitude of the lattice atoms. Approximately 30% of the ions are focused into a peak area with a radius $\leq\rho_{th}$. This focusing may already be restricted by quantum limits and brings us "close" to the size of the nucleus. The focusing of the flux at 35 nm is extremely pronounced, even better than it was expected preliminary. The Monte Carlo simulations led to about 40% of the ions participating in the focusing in an area which is only 4 times larger than the area of the vibrating atom. This means that the "harmonic" area of the channel is much larger then it was initially supposed.

Up to a crystal tilt of 0.125 relative to the $\langle 100 \rangle$ direction of the crystal, the focusing peak remains as sharp as it was without tilting. However, a shift from the center of the channel is observed (Fig. 4). That means, the channel seems to work as an ordinary lens. Nearly the complete area of a channel can be probed with the sharp focus by tilting the crystal: an unique possibility which never occured earlier in atomic collisions. For larger tilt angles the focusing disolves first into two peaks and then disappears. Apart from the peaks there are much weaker concentrations of particles (rainbows, caustics) in the transverse plain which are connected with the non-ideality of the channel as a lens. The weakness of these rainbows is probably connected with the theory of harmonic scattering [15].

Our simulations and also the observed repeated focusing in momentum space [1–3] certify that disturbances connected with the surface of the crystal are negligible in this range of energy and collinearity chosen.

From Figure 5 the maximum of the flux density through an area $\pi \cdot \rho_{th}^2$ is found for an energy of $\approx$150 keV for the impinging ions. Up to 500 keV the maximum flux density decreases by 10% and the FWHM area of the flux density remains smaller than the area of the thermal

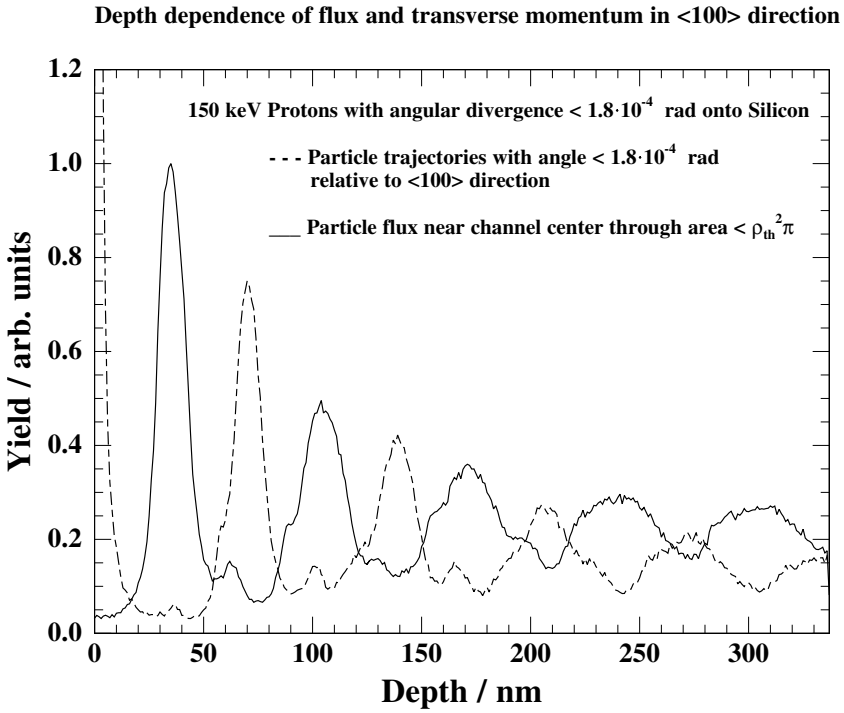

Fig. 2. Flux density and momentum distribution in a ⟨100⟩ channel of a silicon single crystal as a function of depth. The energy of the ions is 150 keV, 10^6 ions are impinging onto an elementary cell with area of $d \times d$ ($d = 0.543$ nm, lattice parameter). The simulations start with a homogeneous irradiation of the surface. The angular divergence for the incident ions relative to the surface normal is $\leq 1.75 \times 10^{-4}$ rad. Flux density and momentum show counterphase oscillations (Liouville's Theorem), which decrease with increasing depth of the ions to an equilibrium condition (normal flux peaking). This decrease results from electronic and nuclear scattering of the ions but mostly from a smearing out of the sharp energy of the impinging ions by the impact parameter dependent electronic energy loss with depth and the resulting energy dependent phaseshift of the focusing lengths for different trajectories. It should be noted that flux density and momentum depth-distributions depend to a certain amount on the chosen interaction potential of the ion-target atom pair (here: Hartree Fock approximation).

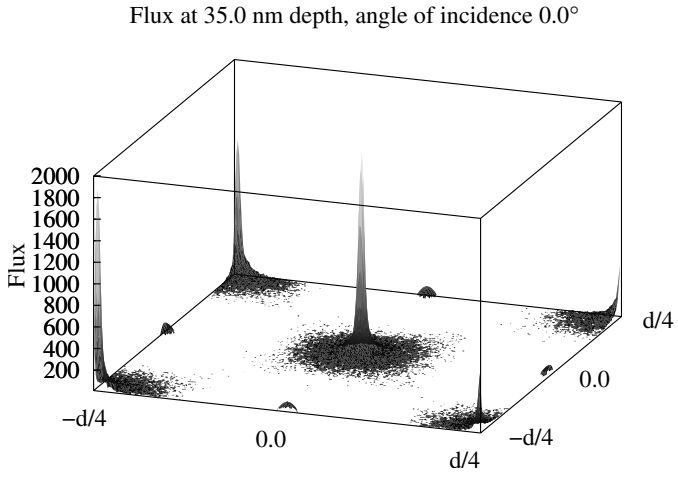

Fig. 3. Focusing of the flux at the depth of its maximum at 35.0 nm in the (100) plane for 150 keV ion energy. The flux density peaks in an area A which is smaller then the thermal vibrational area of the lattice atoms in silicon $A_{th} = \pi \cdot \rho_{th}^2$ ($\rho_{th} = 0.0078$ nm, black semispheres). This results in a factor of more than 500 in the center of the channel for the focused flux density relative to the surface flux density for normal impinging ions.

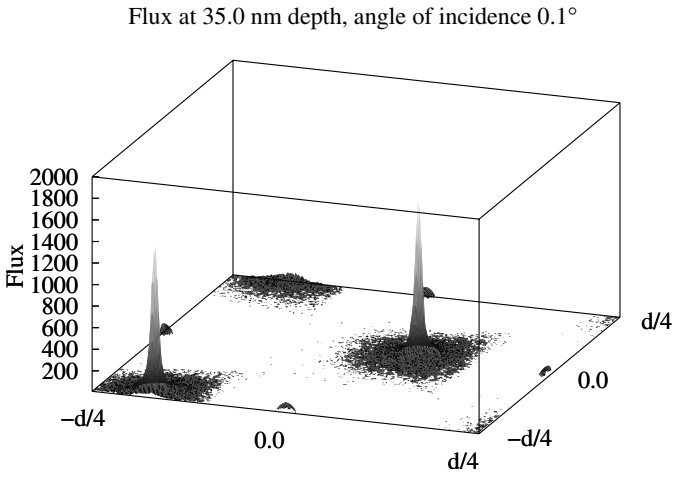

Fig. 4. The crystal is tilted by 0.1 relative to the beam direction and rotated by 13 relative to a main planar channel direction, to avoid planar channeling. Nearly the same sharpness of the focus is observed, whereas the point of focus has moved by ≈0.05 nm out of the center.

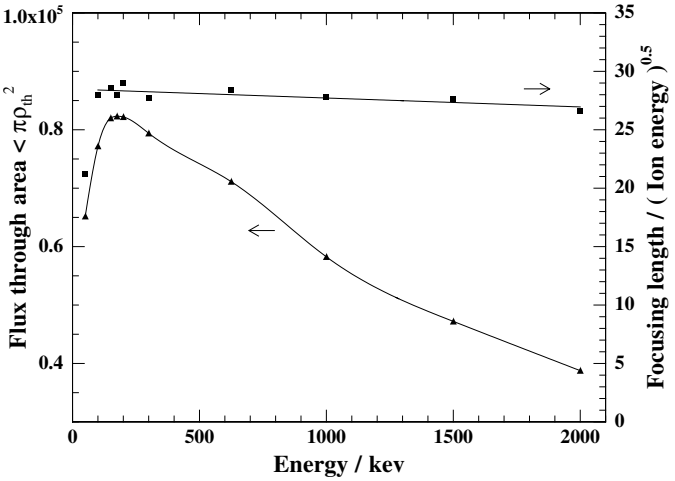

Fig. 5. Energy dependence of the flux through an area of $\pi \cdot \rho_{th}^2$. The highest value occurs for an energy of ≈150 keV for the impinging ions and degrades by more than a factor of two for 2 MeV ions. It should be noted that up to 600 keV the FWHM of the peak is smaller then twice the thermal vibrational amplitude. The upper curve shows the focusing length as a function of energy. This length scales proportional to the ion velocity.

vibrational amplitude. This behaviour reverses for energies larger than 600 keV. The energy dependence of the depth for the first focus scales to a good approximation with the velocity of the ions.

3 Conclusion

To focus a beam of particles down to the size which is smaller than the uncertainty of the elements of the focusing system (the lattice) looks impossible. However, here the repetition of the atoms of the lattice helps by which their positional uncertainty is compensated by the interaction of the beam with large numbers of atoms within the channel. The same result is known from the information theory where it is proven, that one can transmit a signal with arbitrary high accuracy using arbitrary unsave elements. There the possibility is connected with the time-repetition of the signal and the use of some control codes, which is the same idea we use in coordinate space. These methods are the two sides of a more general approach of using rough elements for production of more exact ones.

Many other possibilities, like the use of "semichannels" on the surface of a crystal, rarefied constructions within the solids, channels with decreasing radius, nanometer carbon tubes are upon here.

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