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CHANNELING OF PROTONS IN A <100> Si THIN CRYSTAL: A QUANTUM MECHANICAL APPROACH

DUŠKO BORKA[1], SRĐAN PETROVIĆ[1], VLADIMIR LUKIĆ[2], JEFF TIMKO[3], VESNA BEREC[1] and NEBOJŠA NEŠKOVIĆ[1]

[1]*Laboratory of Physics (010), Vinča Institute of Nuclear Sciences, P. O. Box 522, 11001 Belgrade, Serbia*

[2]*Department of Bioengineering, University of Pennsylvania, Philadelphia, PA 19104, USA*

[3]*School of Physics, University of Sydney, NSW 2006, Australia*

E-mail: dusborka@vinca.rs

Abstract. In this article we analyze the channeling of 2 MeV protons in a <100> Si thin crystal using a quantum mechanical approach. The analysis is based on the numerical solution of the corresponding time-dependent Schrödinger equation in the transverse position plane. The initial wave packet is taken to be of the Gaussian type. We determine the compression coefficient of the wave packet at the superfocusing point in the first rainbow cycle.

1. INTRODUCTION

Demkov and Meyer (2004) performed a classical and quantum mechanical analysis of the spatial focusing of protons of the energy of 1 MeV in the <100> channel of a Si thin crystal in the vicinity of the midpoint of the first rainbow cycle. At this point the reduced crystal thickness, $\Lambda = fL/v_0$, where v_0 is magnitude of the initial proton velocity vector, L the crystal thickness and f the frequency of the proton motion close to the channel axis, equals 1/4. It was assumed that the continuum proton-crystal interaction potential was dominantly cylindrically symmetric and harmonic. They found that the width of the focusing region in the vicinity of the chosen point went below 10 pm, and that the compression coefficient of the proton beam in it went up to several hundred. The effect was named the effect of superfocusing of channeled ions. They suggested that it could be used for subatomic microscopy. The superfocusing effect was also considered by Nešković et al. (2009), who treated it as a crystal rainbow effect (Petrović et al. 2000). They performed a classical analysis of the superfocusing of 2 MeV protons channeled in a <100> Si thin crystal in the vicinity of point $\Lambda = 1/4$. The interaction potential had both the harmonic and anharmonic components. They found that the compression coefficient at the superfocusing point was 47.

2. THEORY

The system we analyze here is a proton beam moving through the <100> channel of a Si thin crystal. The initial proton beam axis coincides with the channel axis. The z axis of the reference frame, being the longitudinal axis, is taken to coincide with the channel axis with the origin lying in the entrance plane of the crystal. The x and y axes of the reference frame are the transverse axes. The interaction of the proton and a crystal's atom is described by the Thomas-Fermi interaction potential in the Moliére's approximation (Gemmell 1974). We apply the continuum approximation (Lindhard 1965). As a result, the Moliére's continuum proton-crystal interaction potential is obtained (Gemmell 1974). The thermal vibrations of the atoms as well as the collisions of the proton with the crystal's electrons are neglected.

The analysis is based on the numerical solution of the time-dependent Schrödinger equation of the system in the transverse position plane, which was obtained by the Crank-Nicholson scheme (Galbraith et al. 1984) improved by us. The initial proton beam is treated as a wave packet of the Gaussian type. The corresponding wave function is $\psi(x, y, t = 0) = [1/(\pi^{1/2}R_s)]\exp[-(x^2 + y^2)/(2R_s^2)]$, where R_s is the initial width of the wave packet, being the radius of the paraxial part of the channel; x and y are the transverse components of the proton position vector and t denotes time. In this part of the channel the continuum proton-crystal interaction potential can be assumed to be cylindrically symmetric and harmonic. If this assumption were valid in the whole channel, the uncertainty of x or y would oscillate between $R_s/2^{1/2}$ and $R_m/2^{1/2}$, where $R_m = \hbar/(2\pi mfR_s)$, with m being the proton mass and ħ the reduced Planck constant (Demkov and Meyer 2004). The upper level, $R_s/2^{1/2}$, would be reached for t = 0, T/2, T, ..., corresponding to Λ = 0, 1/2, 1, ..., and the lower level, $R_m/2^{1/2}$, for t = T/4, 3T/4, 5T/4, ..., corresponding to Λ = 1/4, 3/4, 5/4, ..., respectively. For Λ = 1/4, 3/4, 5/4, ... the wave packet is superfocused. We are interested here in the superfocusing effect at point Λ = 1/4, the corresponding time being t = T/4, when the interaction potential is neither cylindrically symmetric nor harmonic. As it has been said above, the interaction under consideration is described by the Moliére's expression.

3. RESULTS AND DISCUSSION

The initial proton energy is taken to be 2 MeV. We assume that the crystal's atomic strings defining the channel intersect the x and y axes. The number of atomic strings of the crystal is 16, i.e., we take into account the atomic strings lying on the two nearest square coordination circles. The value of f is 5.94×10^{13} Hz. It is determined from the second-order terms of the Taylor expansion of the continuum proton-crystal interaction potential. The value of L corresponding to Λ = 1/4 is 82.6 nm. We choose that the paraxial part of the channel is determined by R_s = 33.9 pm, being equal to one quarter of the distance between the channel axis and each of the atomic strings defining the channel.

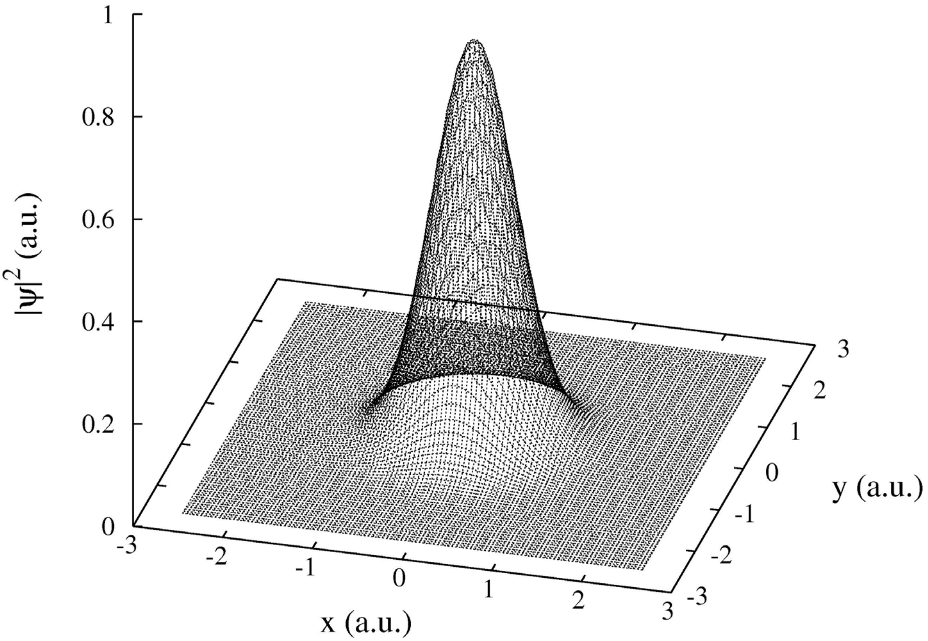

Figure 1: The modulus of the wave function squared corresponding to the initial proton beam, at t = 0.

Figs. 1 and 2 give the moduli of the wave functions squared corresponding to the initial proton beam, at t = 0, and the proton beam at the superfocusing point, at t = T/4 (Λ = 1/4). As it is expected, in the latter case the amplitude of the wave packet is much larger and its width much smaller than in the former case. The ratio of these amplitudes is 25. The full-width at half-maximum of the former wave packet is $\Delta\rho_s$ = 1.068 a.u. = 56.6 pm. The full-width at half-maximum of the latter wave packet along line x = 0 or y = 0 is $\Delta\rho_{m1}$ = 0.212 a.u. = 11.2 pm, while its full-width at half-maximum along line y = x is $\Delta\rho_{m2}$ = 0.146 a.u. = 7.8 pm. This result confirms the finding of Demkov and Meyer (2004) that the width of the wave packet at the superfocusing point was much below the Bohr radius, which lead them to the conclusion that the superfocusing effect could be used for subatomic microscopy. We take that the compression coefficient of the proton beam at the superfocusing point is $\kappa = [\Delta\rho_s^2/(\Delta\rho_{m1}\Delta\rho_{m2})]$. Hence, κ = 37. This value is smaller than the values of κ obtained by Demkov and Meyer (2004) and by Nešković et al. (2009). We attribute this difference to the anharmonic part of the continuum proton-crystal interaction potential, which was neglected in the estimations of those authors.

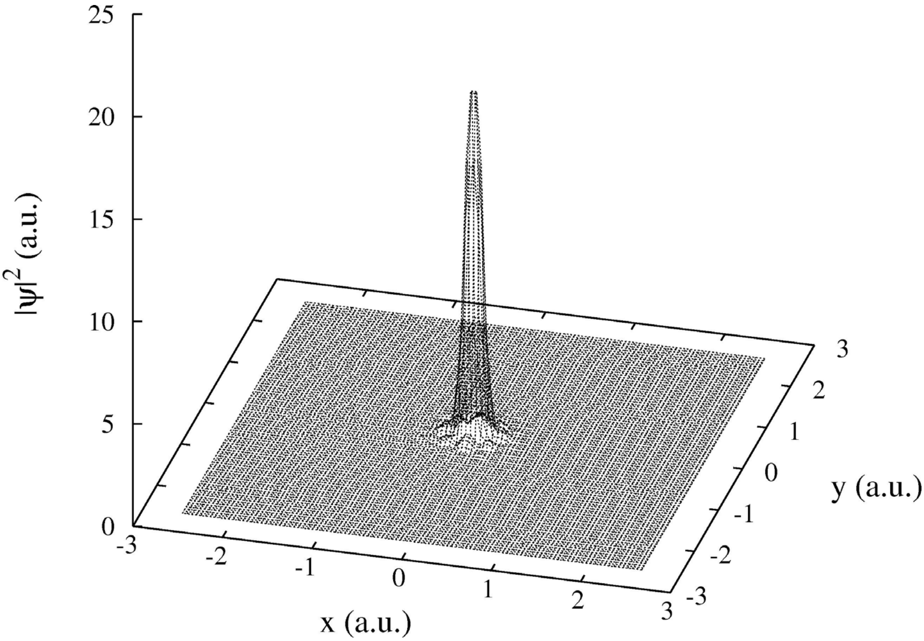

Figure 2: The modulus of the wave function squared corresponding to the proton beam at the superfocusing point, at t = T/4 (Λ = 1/4).

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