ПРЕДПРИЯТИЕ ГОСКОРПОРАЦИИ "РОСАТОМ"

ФГУП "ВСЕРОССИЙСКИЙ НАУЧНО-ИССЛЕДОВАТЕЛЬСКИЙ ИНСТИТУТ АВТОМАТИКИ им. Н.Л.Духова"

Modeling of channeling effect for deuterons in a TiD_2 crystal

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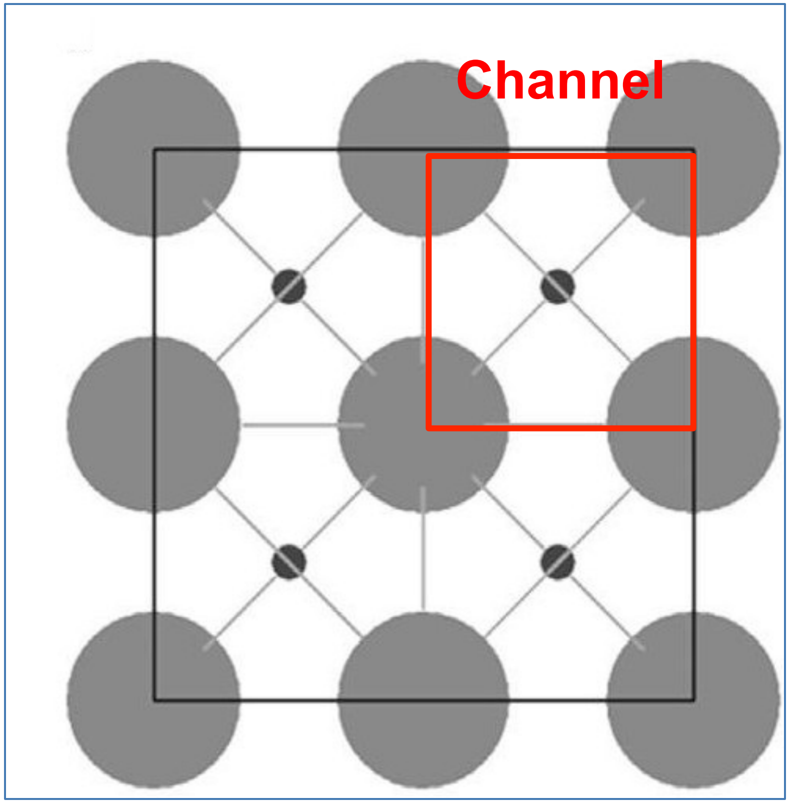
Problem statement

- dd reaction enhancement was experimentally observed in textured targets of titanium deuteride at ultralow energies [1]
- This effect can not be fully described by the electron screening due to unphysical U_e = 131 eV (15 eV in adiabatic models)



TiD_2 lattice in [1 0 0] direction

Development of a 3D channeling model for deuterons in TiD_2 crystal

[1] NIMA 764 (2014) 42-47

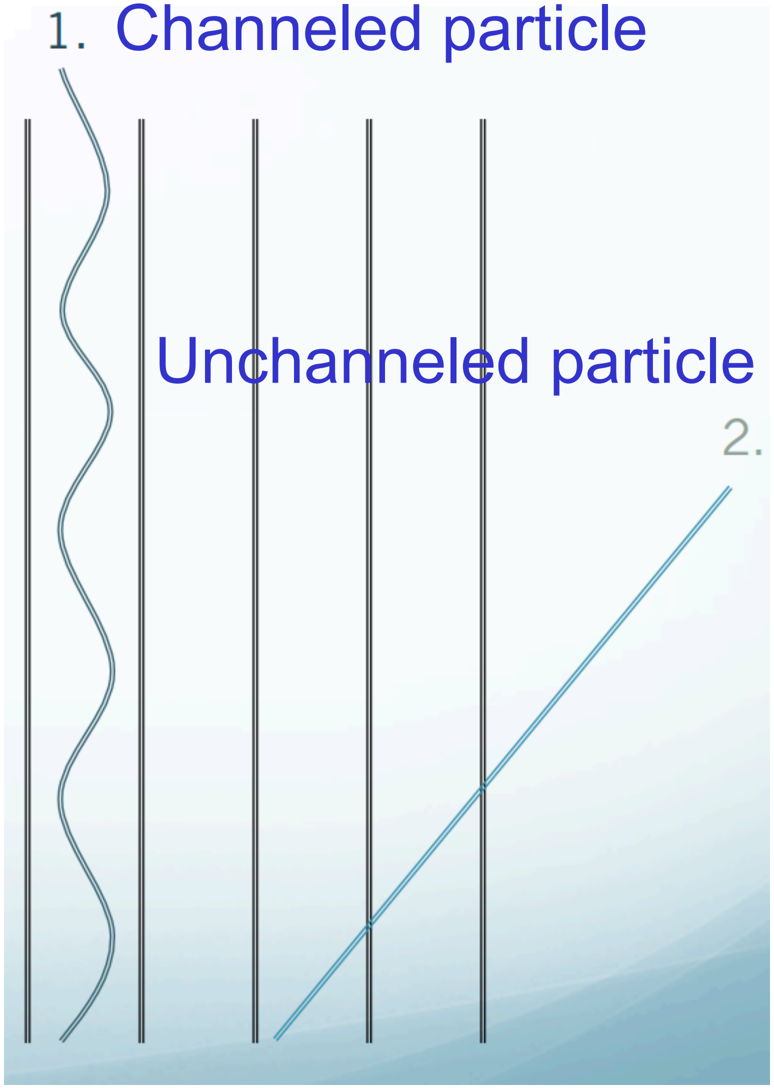
Lindhard potential

Y(x) - continuous plane potential

- Scattering angles are assumed to be small
- Collisions are correlated
- Classical picture can be used
- Idealized lattice

Particles channeling along planes with a normal i must obey:

$$\frac{p_i^2}{2m} < Y_{\max}$$



Model assumptions

• Channeling deuterons has a lower energy loss. This defines higher thickness of the effective target.

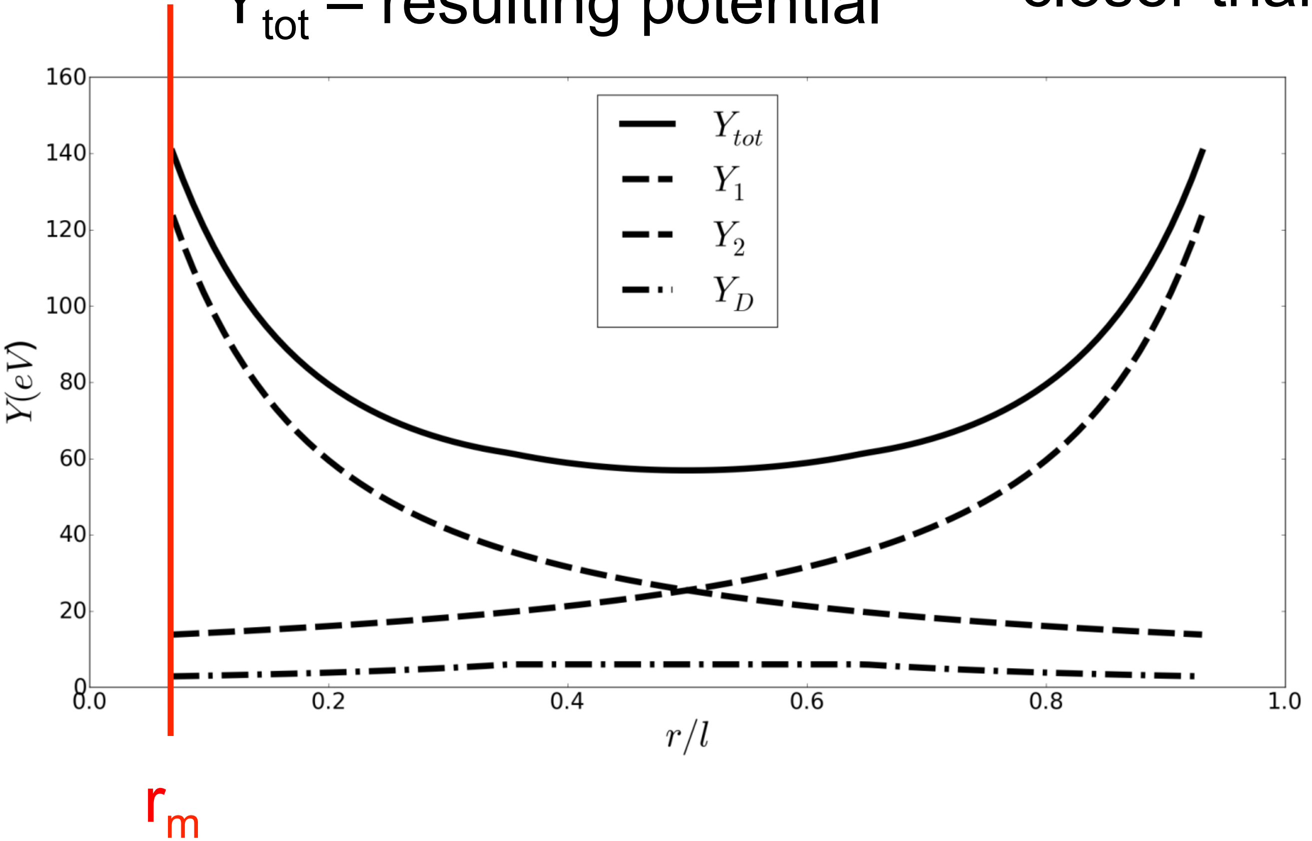
• Average energy loss due to the electronic stopping power is proportional to the lower electronic density.

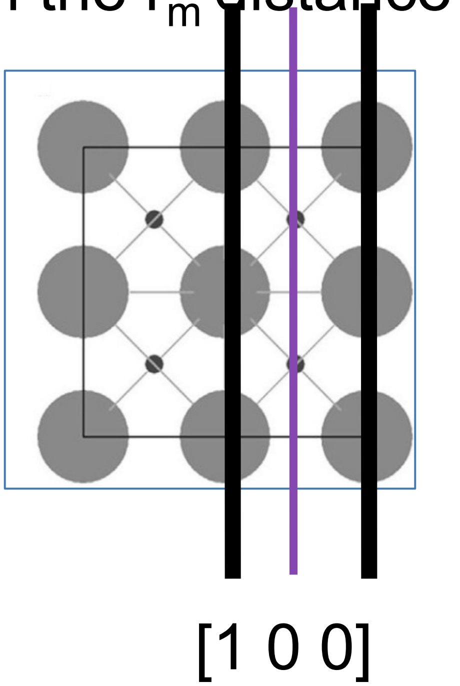
• Channeling deuterons are focused by titanium atoms to the area of target deuterons. This increases the effective deuteron flux density.

Plane potential

Y_D - deuterium plane
Y_1,Y_2 – titanium planes
Y_{tot} – resulting potential

Channeled particle can not approach to a plane closer than the r_m distance

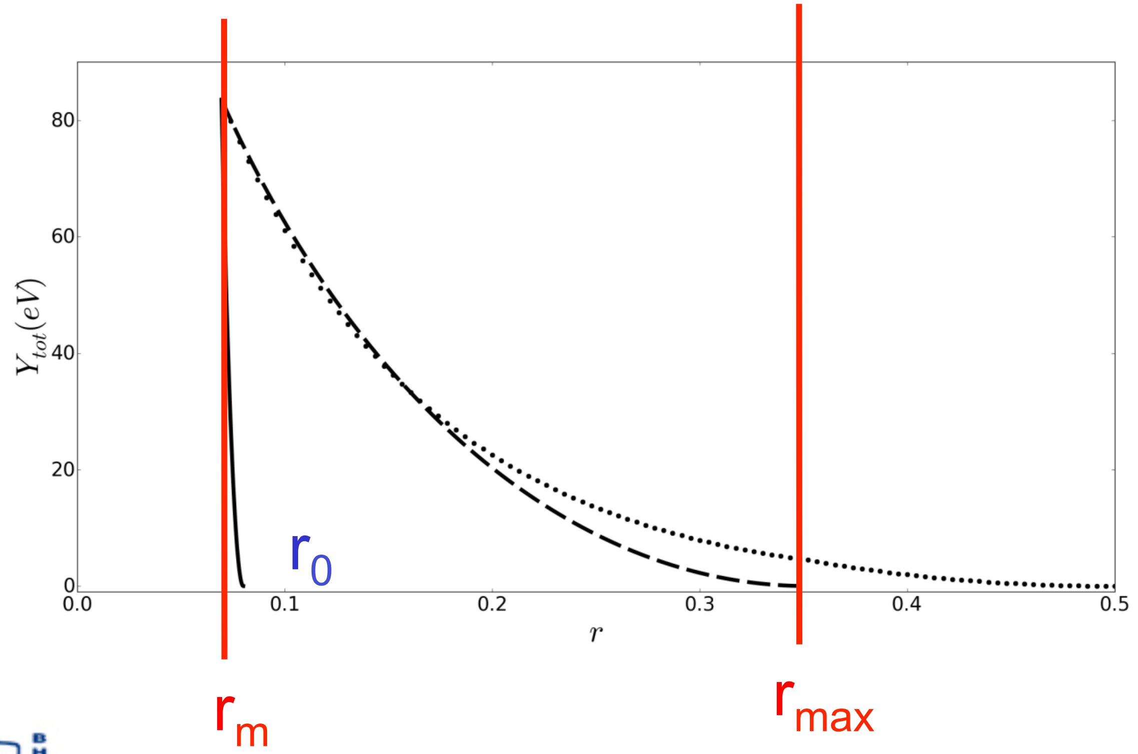




Renormalization of the potential and the r_0 parameter

The resulting potential was renormalized.

Its width r_0 ($r_m < r_0 < r_{max}$) was varied to match the experimental data.

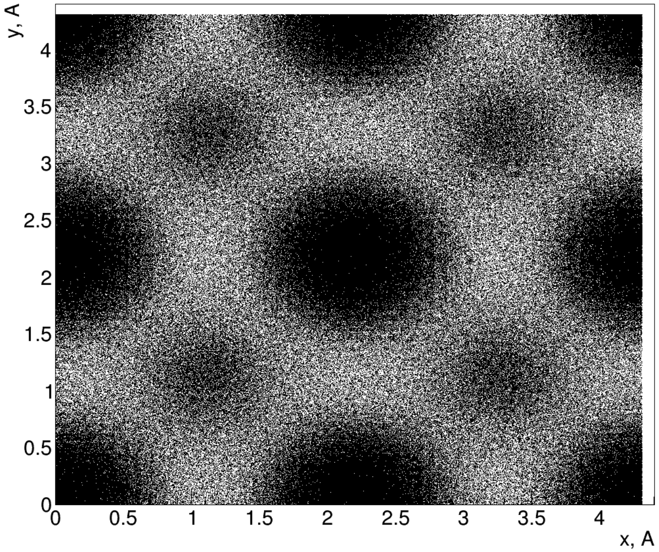


Modification of the stopping power

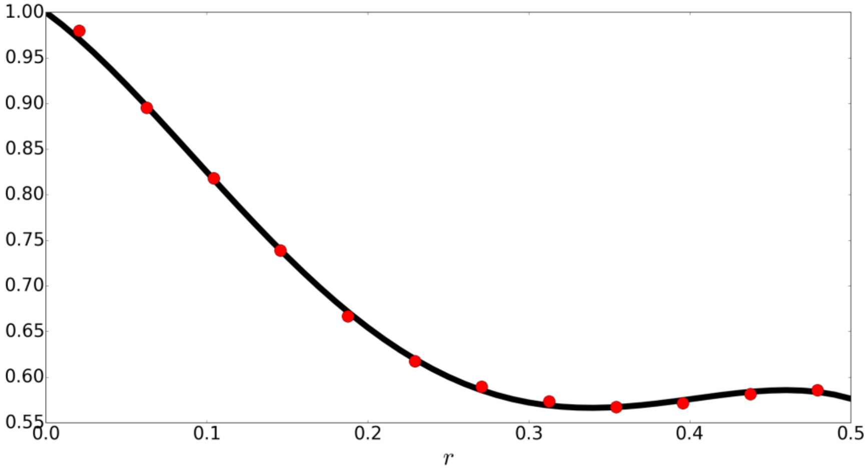
$S = S_e + S_n$

S_e is proportional to the average electronic density along the track

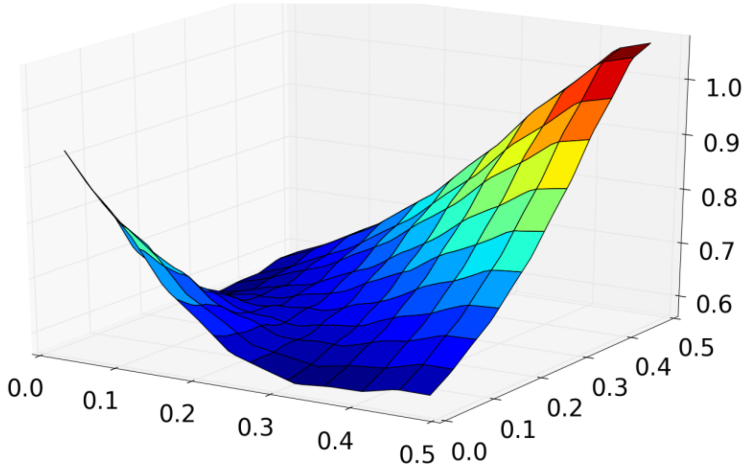
$$S_n^{chan} = S_n^{amorph} \cdot \frac{2Z_D}{2Z_D + Z_{Ti}}$$



3D TiD_2 electronic density



1D normalized electronic density

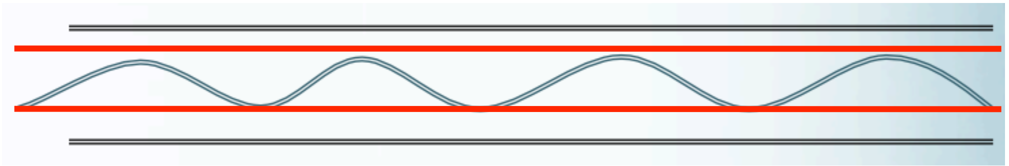


2D normalized electronic density

Flux compression

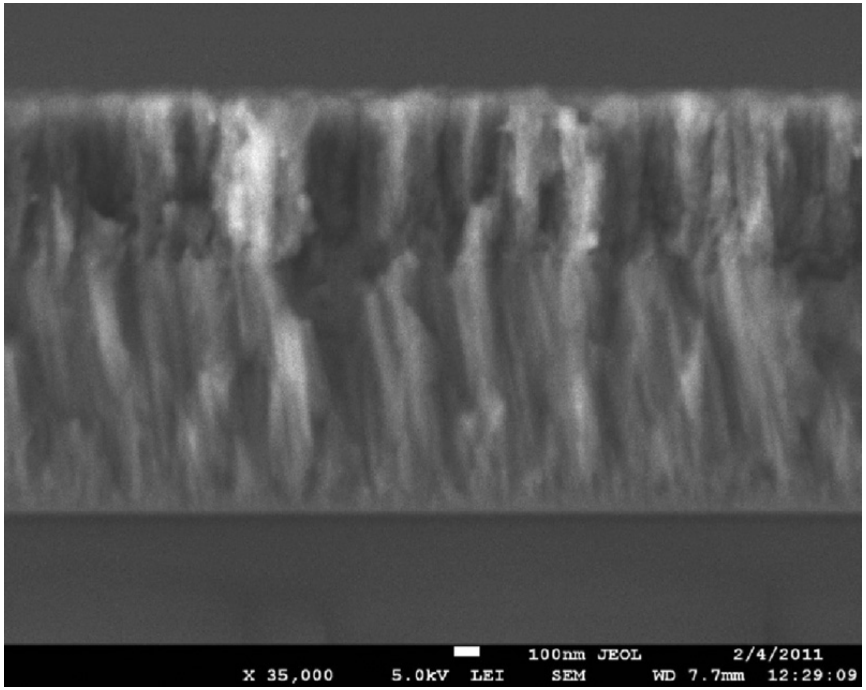
$$\frac{p_i^2}{2m} = Y(x_{\min}) \longrightarrow$$ x_{min} – minimal distance to the Ti plane.

Density of the channeled particles flux increases reverse proportional to the available volume.



Variation of the r_0 parameter changes the flux compression effect and can effectively take into account the imperfection of the crystal.

Multiple scattering



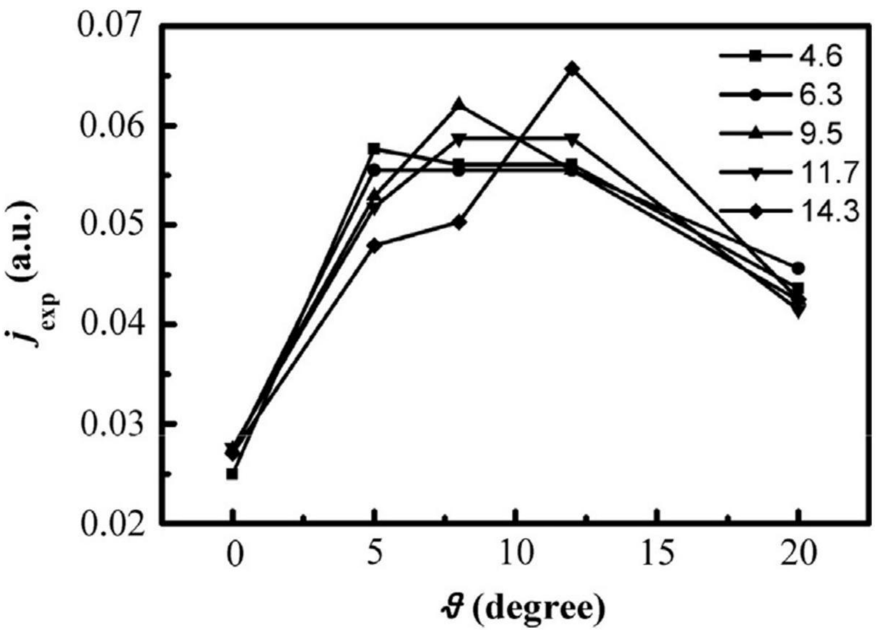
Electron microscope image of a cleavage of the TiD_2 [NIMA 764 (2014) 42-47]

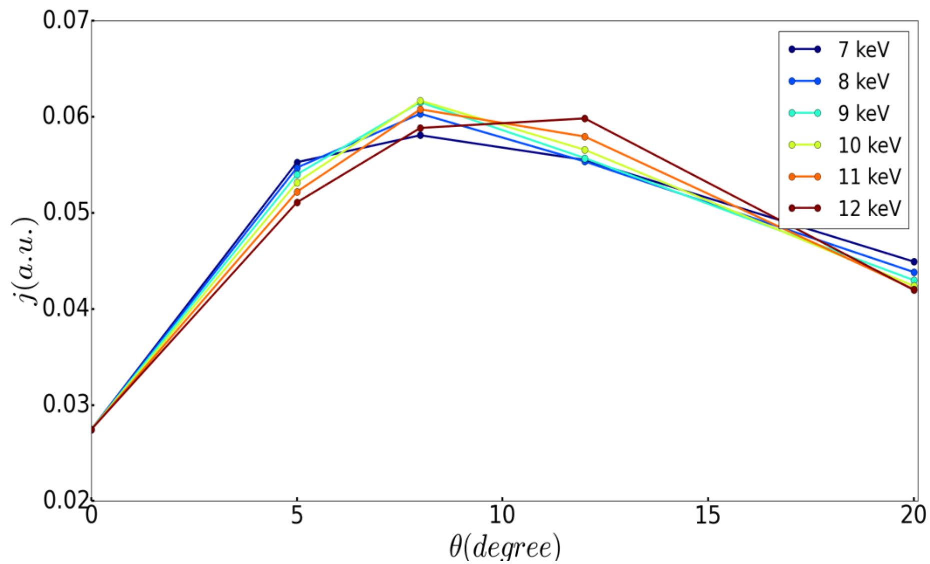
Geant4 multiple scattering for

- Unchanneling particles
- Channeling particles

Approximation of angular distributions

Experimental angular distributions were interpolated for six energies 7 – 12 keV.



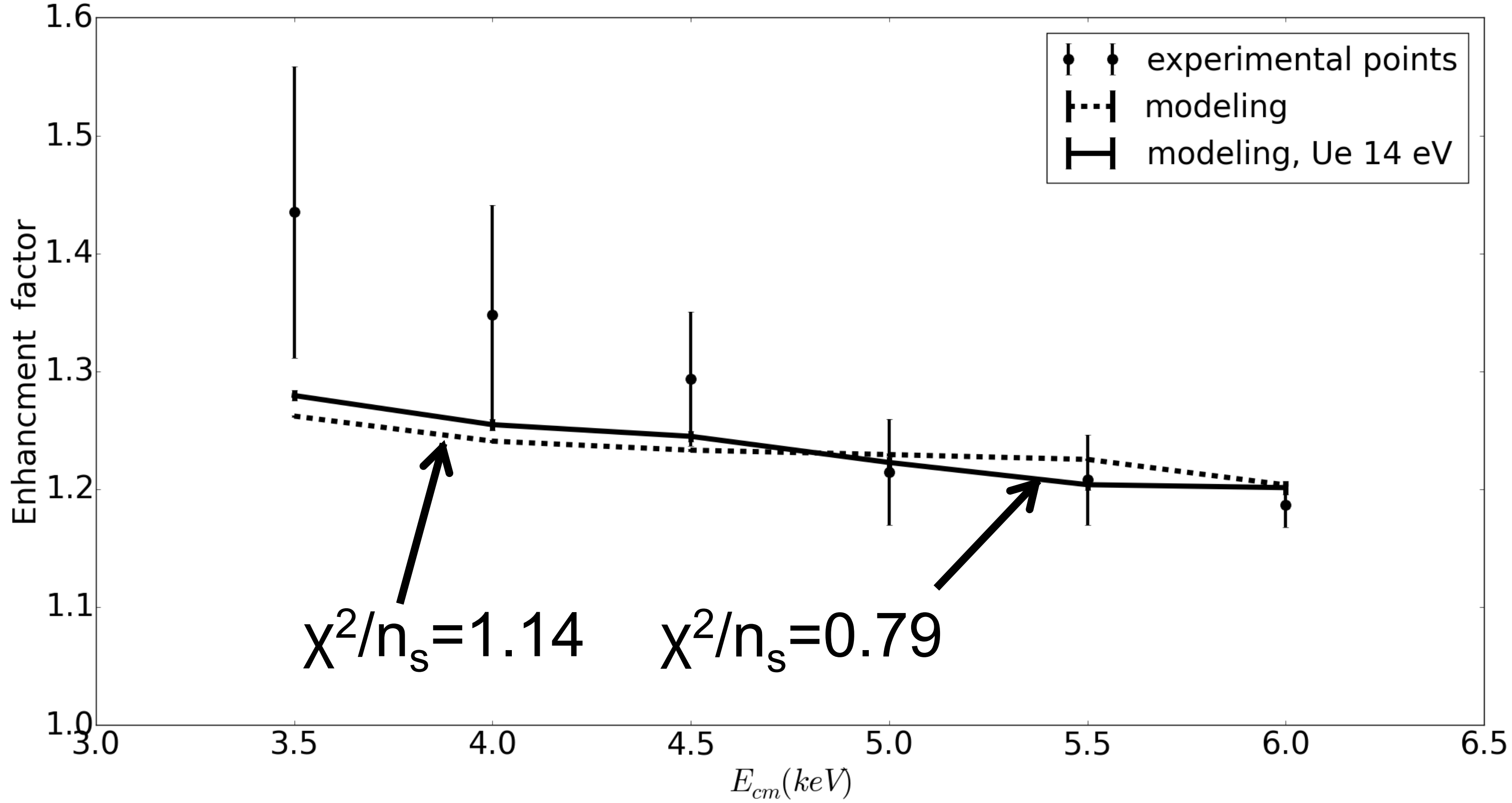


Experimental angular distributions [NIMA 764 (2014) 42-47]

Interpolated angular distributions

Validation

Comparison of the enhancement factors calculated by TPT-EM with and without electron screening (solid and dashed curves respectively) and the experimental values



Conclusion

The developed TPT-EM model describes experimental data for titanium deuteride. If the crystal is perfect the effect is expected to be a few times bigger.

Further development

- Develop TPT-EM multiple scattering process for channeling particles
- Develop TPT-EM dechanneling process

Thank you