Calculation of Muon Depth Distributions in Thin Film Single Crystals

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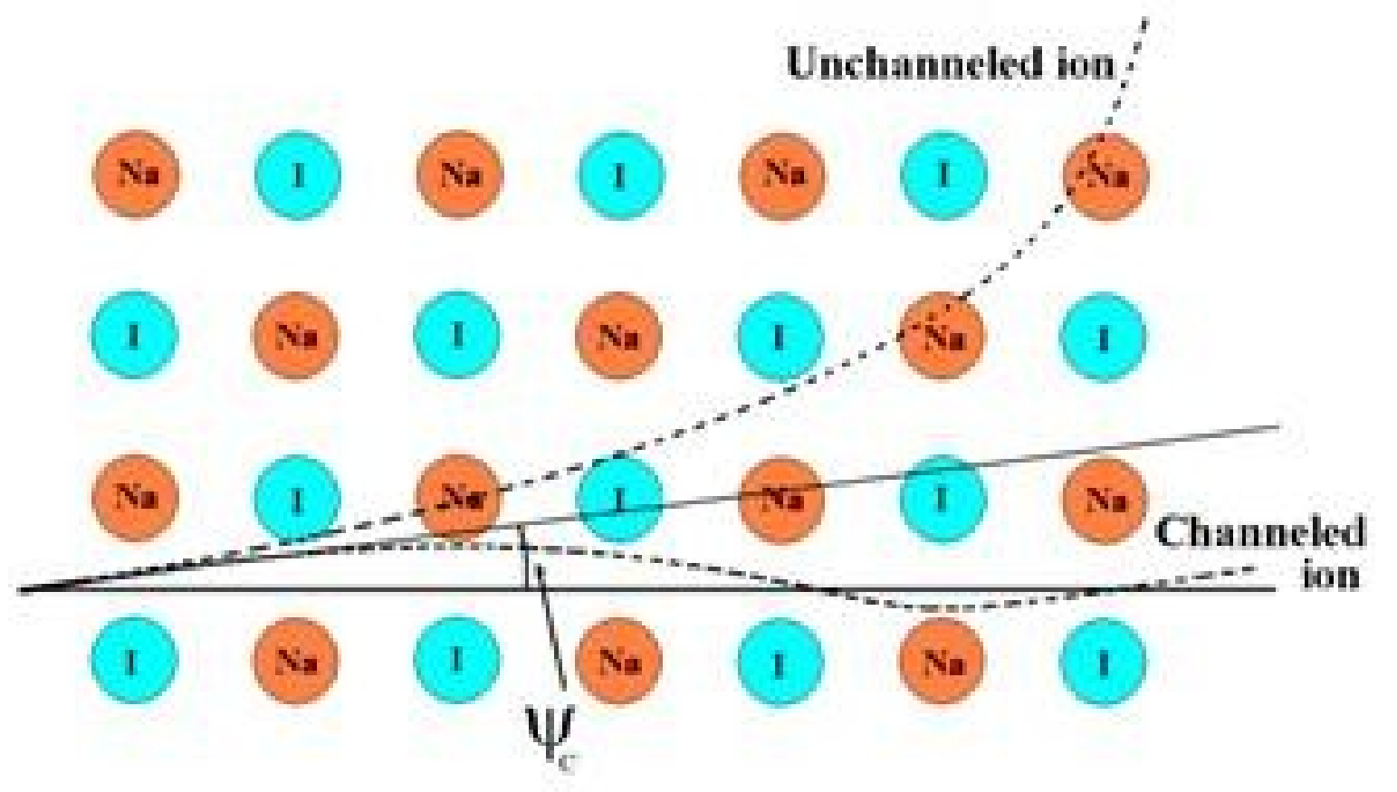
A computer code, with acronym MUSCLE, is written to treat the simulation of muon transport and stopping in crystalline thin film samples. While programs such as TRIM have proven useful for this purpose in amorphous samples, channeling associated with crystalline material can alter the stopping spatial distribution with greater depths being reached and the overall shape being also affected. For bcc iron we compare our results to those of a Monte Carlo program from Oak Ridge National Laboratory, MARLOWE, which is also designed for crystalline material, and to distributions determined from TRIM. Finally we note that with channeling transport out of the thin films is more likely and is discussed.

Muon Stopping Distribution

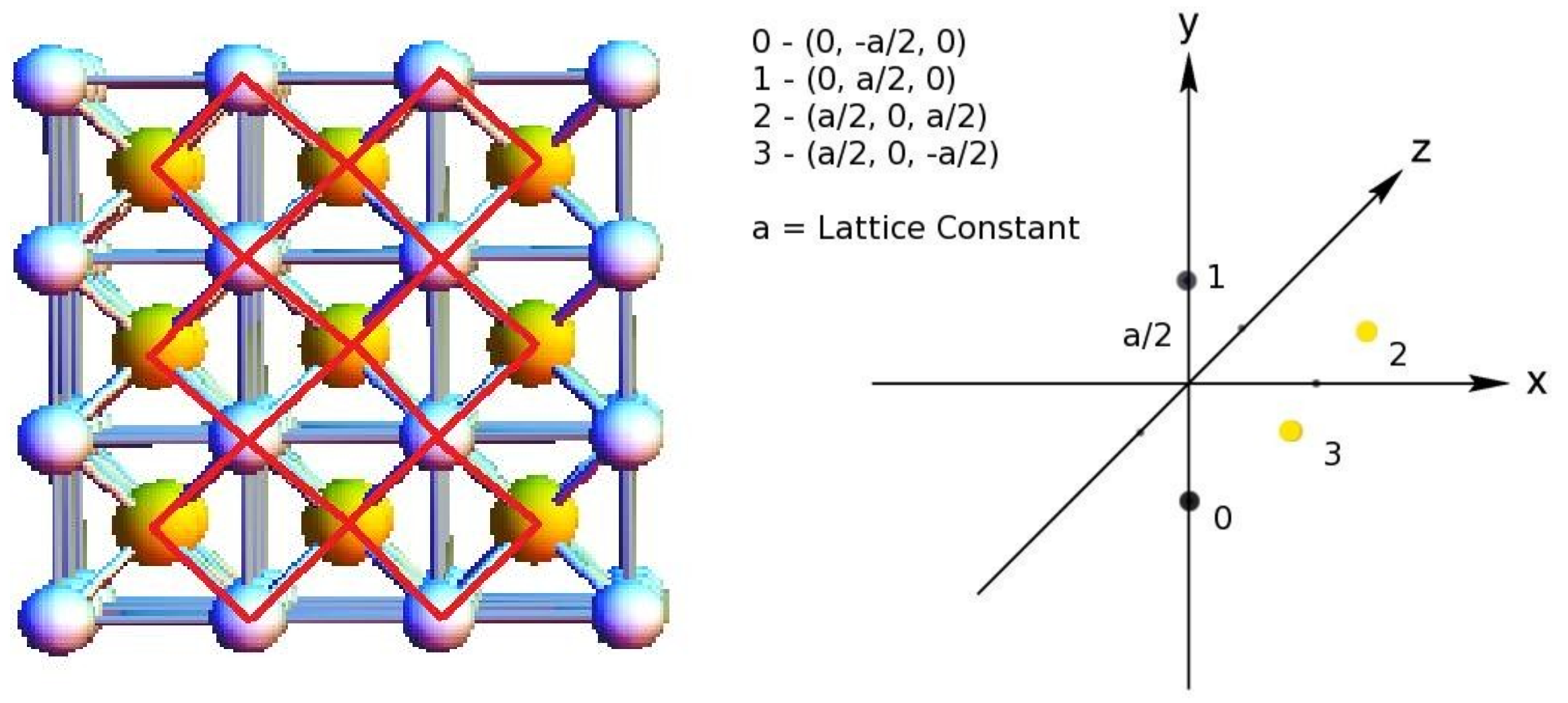
In order to determine the depth distribution of stopped muons in a target layer, the program named TRIM is used by some researchers. TRIM is used to simulate passage of ion beams through amorphous samples using the Binary Collision Approximation (BCA) method. However, if we consider the crystalline structure of a material, channeling of particles may affect the shape of the spatial distribution by leading some particles to reach greater depth, or transmit out of a thin film. In a multi-layered target, this may affect the combined stopping distribution. In order to investigate this issue, we have written a collection of programs called MUSCLE (MUonS Cascade at Low Energy) that include an approximation scheme to detect channeling of muons in a crystal and a molecular dynamics model that gives a better estimate of the channeling process. The results from MARLOWE (another BCA program) are also included for comparison.

Channeling

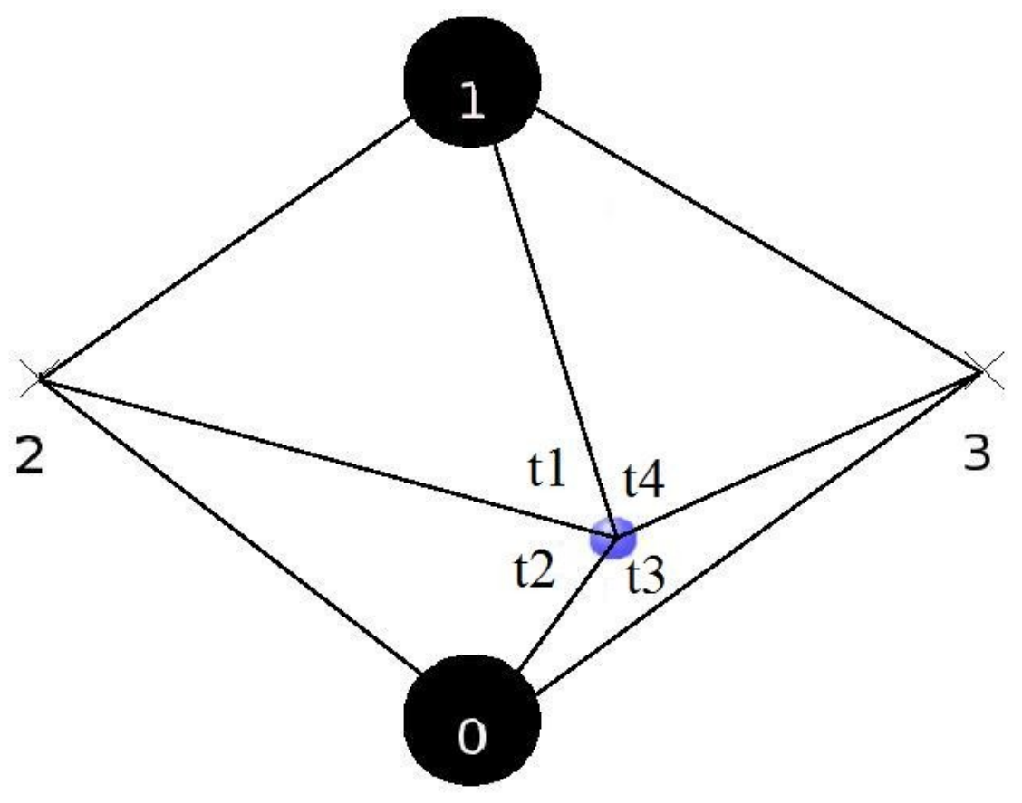
Channeling is the phenomena of constrained ion motion along crystallographic axes and planes due to which ions manifest an anomalous deep penetration. Our goal is to treat the target as a crystal and investigate the effect of channeling on stopping distribution.



Preliminary Investigation

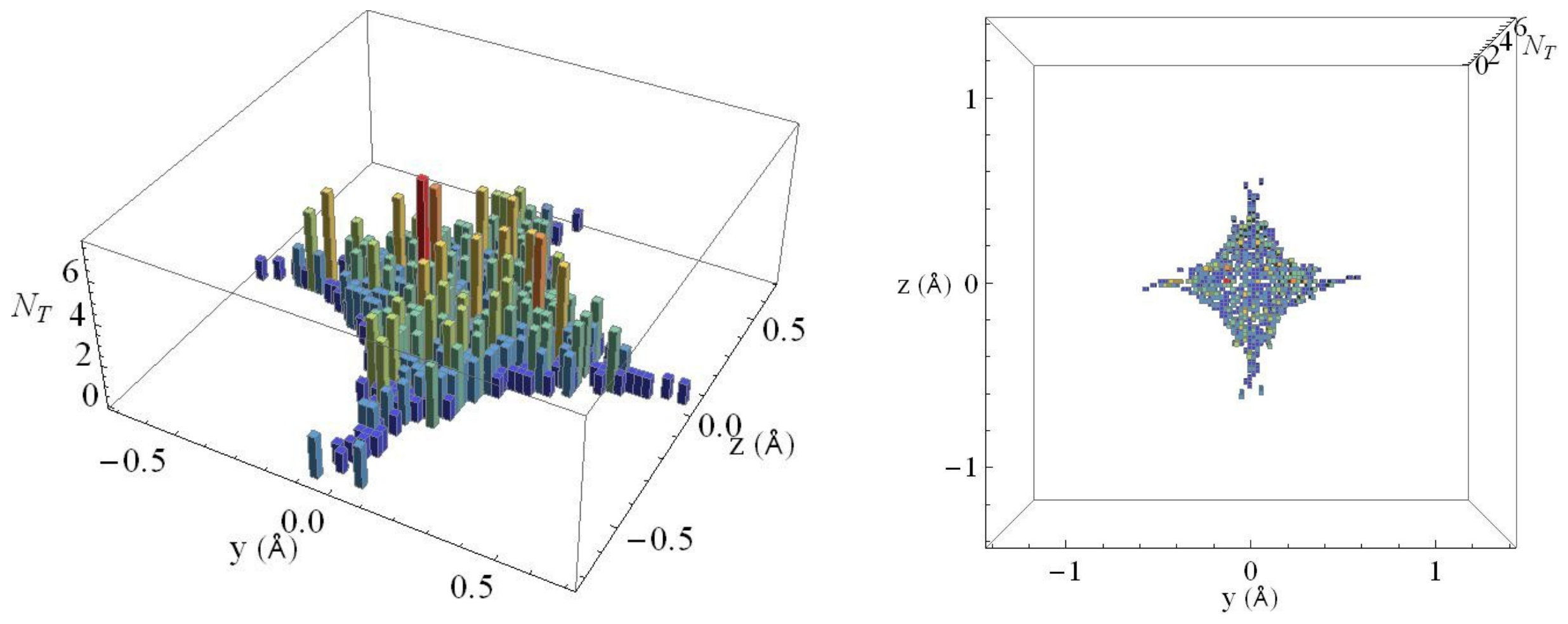


A potential channeling region in a bcc crystal.

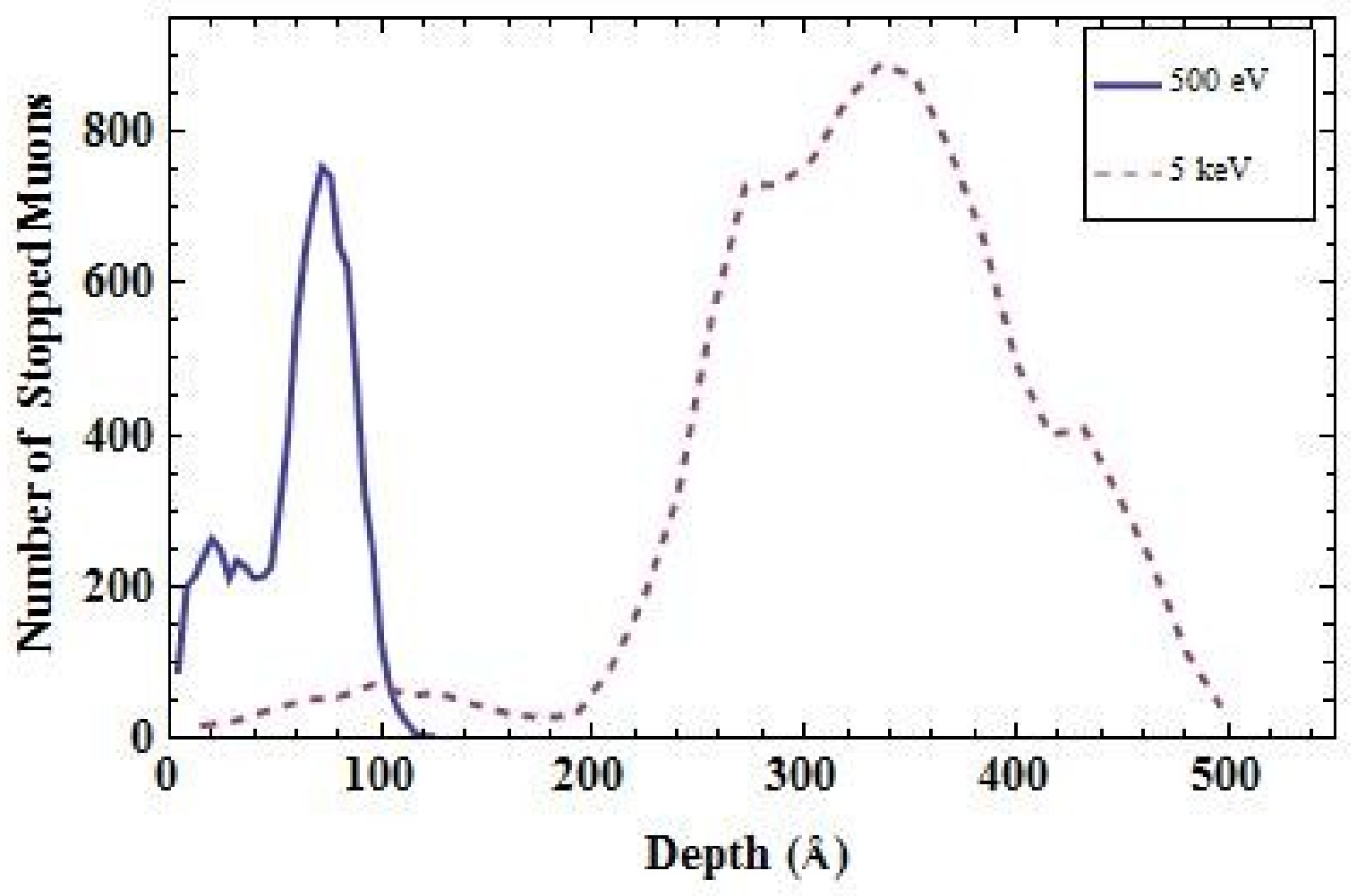


A point-in-polygon algorithm Is used to determine whether a muon stayed inside the channeling region. The angles t1, t2, t3 and t4 should add up to (2π, 0) if the muon is (inside, outside) of the region.

The simulation for 500 eV normally incident muons on iron shows that around 20% of the muons remain in the channeling region before reaching 10 nm. The shape of the actual channeling region is depicted correctly by the histogram.



MARLOWE Simulations



MARLOWE simulations for 500 eV and 5 keV normally incident muons show evidence of channeling. While the average depth of muons are comparable to what TRIM estimates, the 500 eV muon distribution has two visible bumps not seen for TRIM. The first bump is not so visible for 5 keV muons, i.e. higher energy muons have greater chance of departing from channels, and hence, the distribution looks much similar to what TRIM produces.

Molecular Dynamics Model

In order to take account of simultaneous scattering from surrounding atoms (which may capture the channeling process effectively), we have written a basic molecular dynamics algorithm.

$$M_i \frac{d^2\vec{r}_i(t)}{dt^2} = \sum_{j=1}^{N} \vec{F}_{ij} = \vec{F}_i(\vec{r}_i(t))$$

The force is derived from a potential function.

$$M_i \frac{d^2\vec{r}_i(t)}{dt^2} = \vec{F}_i(\vec{r}_i) = -\sum_{j\neq i} \nabla V_{ij}(\vec{r}_{ij})$$

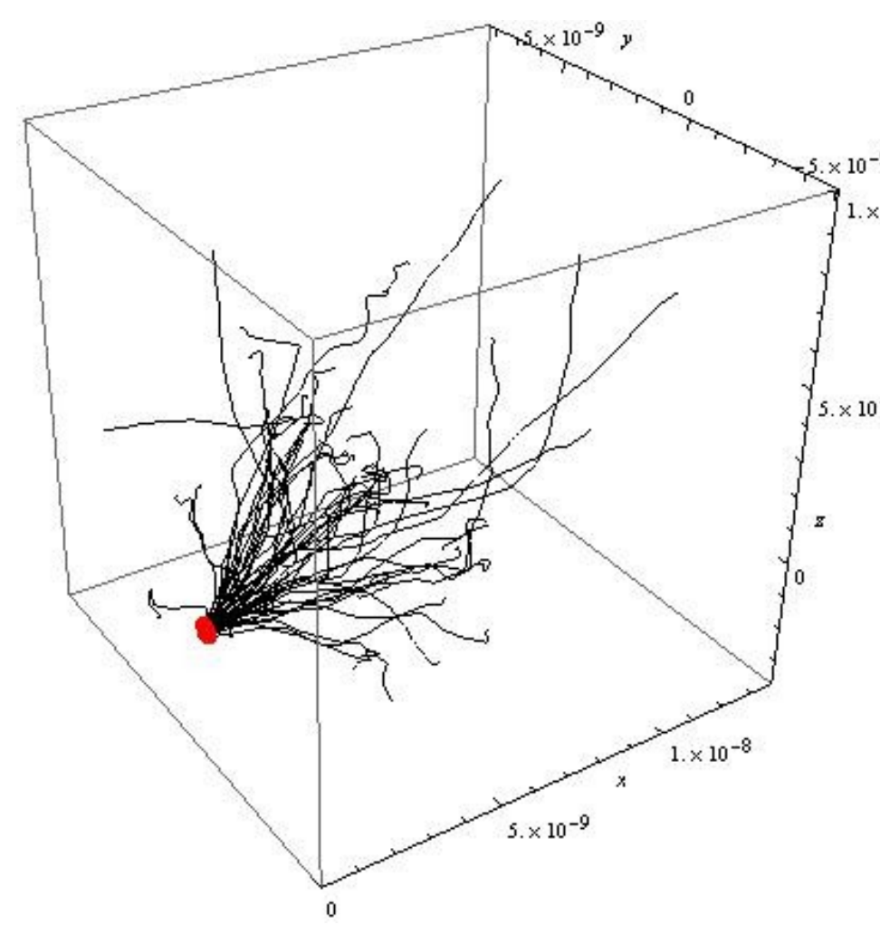
The Born-Mayer potential function is used.

$$V(\vec{r}) = A_{BM}\, e^{-\frac{|\vec{r}|}{a_{BM}}}$$

Electronic stopping is implemented by calculating the stopping cross section S_e, and reducing the velocity of muons by

$$\triangle v = \triangle t\, \frac{S_e}{M_m}$$

Muon Trajectory using Molecular Dynamics



Beam trajectory generated by the MD simulation for 500 eV muons normally incident on a body centered cubic crystal (iron).

Comparison between MUSCLE (MD) and TRIM

Program	Average Range (angstroms)	Maximum Range (angstroms)	Transmitted Particles
MUSCLE (MD)	68.85	709.8	376
TRIM	70.49	339.6	64

The simulations were run for 10000 normally incident muons with 500 eV energy. Muons were assumed to be transmitted if they penetrated over 200 Ǎ. Although the maximum range and number of transmitted particles is higher for MD (an evidence of channeling), no alarming deviation from TRIM is found.

Conclusion

- MD and multiple collision BCA models (MARLOWE) are more accurate compared to single collision BCA models (TRIM) in terms of simulating the channeling effect.
- Channeling does not have considerable effects in the final stopping distribution. Hence, using TRIM is fine for the purpose of muon beam physics simulations.
- Higher number of transmitted particles (compared to TRIM) due to channeling may indicate a possible change in the shape of the combined stopping distribution for a multi-layer thin film target. However, such a chance is slim considering the small percentage of transmitted particles.