The stopping distribution of low energy $^8Li^+$

W.A. MacFarlane
Chemistry Department, University of British Columbia, 2036 Main Mall, Vancouver BC, V6T 1Z1
(Dated: April 2004)

This is meant to be an introduction to this important aspect of using β-NMR as a depth-resolved magnetic probe. What do we know about the stopping distribution of Li? Why do we need to know the stopping distribution? How to use the stopping distribution? Disclaimer: Just because it's nicely typeset doesn't mean it's error-free.

PACS numbers:

I. THE IMPORTANCE

To make the depth profiling capability of β-NMR *quantitative*, it is essential to have a complete understanding of the stopping distribution of the probe, $^8Li^+$ (with kinetic energy 10 eV - 30 keV). For example, Fig.2 shows the bias scan of the β-NMR resonances at 280 K in the epitaxial heterostructure GaAs⟨100⟩ 20Å Fe/ 800 Å Ag 40 Å Au. At intermediate bias, the stopping distribution might be qualitatively as shown in Fig.1. In order to get a meaningful fit of the resonance at the Larmor frequency, it is important to know how much of this resonance could be due to ^8Li stopping in the substrate, for example. Even if all the ^8Li stops in the Ag layer, the implantation depth profile will cause a nonuniform sampling of any depth dependant phenomena in the Ag layer.

A great deal is known about the stopping of ions in matter[1,2], primarily because ion beam irradiation is a technique used in industrial semiconductor manufacturing, however, the energies we are interested in are typically much lower than those that have been studied.

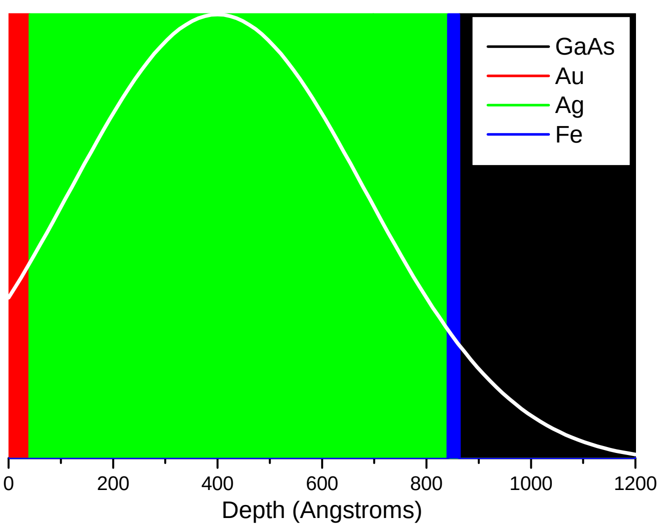

FIG. 1: A to-scale representation of the thin-iron thick-silver heterostructure with a representative gaussian stopping distribution superposed. The heterostructure is a capping layer of 20 monolayers of Au on 400 ML of Ag on 14 ML of Fe on the GaAs substrate.

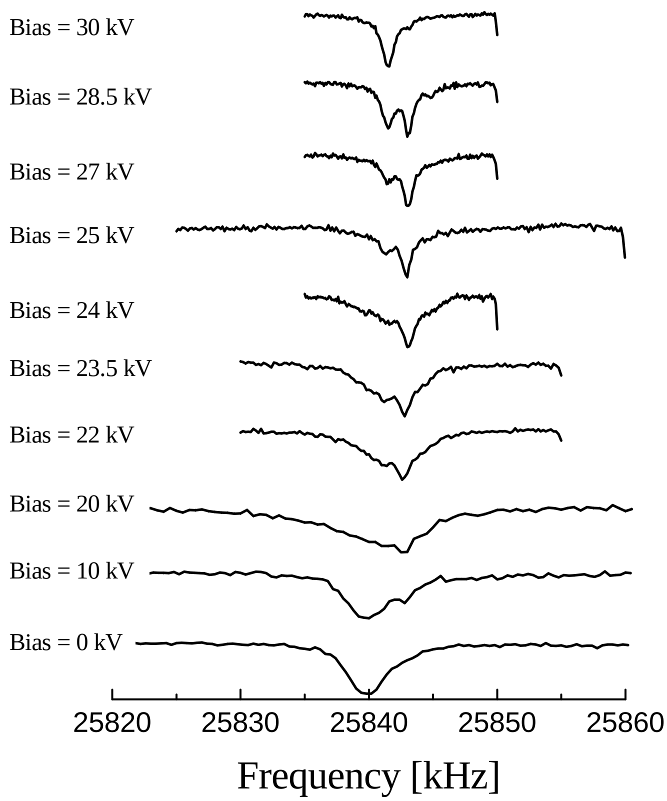

FIG. 2: Platform bias scan of the resonances of ^8Li in the heterostructure shown in Fig. 1. Figure courtesy of A.N. Macdonald and T.A. Keeler.

Monte carlo computer programs to model the stopping of ions have been developed and extensively compared with experiments. Experiments implanting radioactive probes are one such test, but also one can depth profile implanted ions using techniques like SIMS and Auger Spectroscopy in combination with a sputter gun (for hole-digging). One such program is SRIM[3]. This appears to be an offshoot of an original program called TRIM. We are currently using a modified version of TRIM, called TRIM.SP (modified by LEμSR[4]). These programs typically *do not* include the effects of channeling which can have significant effects on the stopping distribution in **crystalline** films. They do include density and nuclear charge (atomic number Z) effects, but no microstructural effects of the lattice. The output of such programs

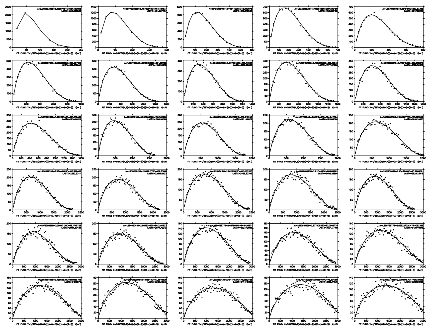

FIG. 3: Predicted stopping distributions from TRIM.SP for various ^{8}Li energies (points) and beta distribution fits (lines) (Courtesy D. Wang).

is a set of points scattered about a theoretical stopping distribution. Presumably with enough simulations these points would converge on a smooth curve. The physical processes important in stopping ions are given in refs[1,2]. Zaher has agreed to show us how to operate TRIM.SP sometime in the near future.

One question immediately arises, what is a good phenomenological functional form for the stopping distribution? If we can find a nice parametrization of the predicted distribution, then we could use it to sort out examples, such as the above, in a convenient way. I will show some examples of this in the next section. Typically the stopping distribution is approximated as a gaussian, but often the distribution is not that symmetric, particularly when there is a channeling peak which can make the distribution bimodal.

As an example, Dong Wang finds the stopping distribution for ^{8}Li in $NbSe_2$ is not well-described by a gaussian and has parametrized it instead using the beta distribution:

$$f(z;a,b) = \begin{cases} c\frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}\tilde{z}^{a-1}(1-\tilde{z})^{b-1}, & \text{for } z \in (0,1) \\ 0, & \text{elsewhere,} \end{cases} \quad (1)$$

where $\tilde{z} = z/z_0$ is a dimensionless normalized depth. This distribution has a mean value $a/(a+b)$ and a variance $ab/(1+b)^2(a+b+1)$[5]. The fits to the monte carlo data for ^{8}Li stopping in $NbSe_2$ are shown in Fig.(3). One can see that the fits are quite reasonable. To my knowledge, there is nothing fundamental in the use of the beta distribution, it is just a versatile phenomoenological form. Another question that this suggests: is there a natural function to use (beyond the gaussian)?

The monte carlo programs involve phenomenological parameters which can be adjusted to match experiment. Some work has been done using ^{7}Li in Si for example[6], but for our energy range, it may also be necessary to more extensively test the predictions of such programs using β-NMR (along the lines of refs[4,7]) and possibly have the programs modified if necessary.

Once we've established the stopping distribution, we can use it.

TABLE I: Beta Distribution fits to the TRIM.SP implantation distributions predicted for $NbSe_2$, courtesy D. Wang.

z_0	a	b	c
36.6345566	2.26532368	9.99987784	531.450668
44.4667757	1.97723688	5.46752944	464.461677
61.2272566	1.91213954	4.97494402	348.940872
75.2823165	1.93321953	4.70395483	287.640109
92.7180259	1.98794684	4.8315186	233.83368
98.9102647	1.89046751	4.04500465	225.227106
112.820278	1.90773033	3.94678169	201.181766
123.054994	1.84876239	3.57720408	183.514615
137.737008	1.90512292	3.70553565	166.68641
150.876939	1.97880687	3.71901639	152.976878
163.490127	1.85160299	3.48256345	143.172482
170.094569	1.82135816	3.23726676	138.365966
182.149078	1.89645047	3.23671691	130.017247
191.204039	1.8776904	3.05018485	123.831776
201.694888	1.83905356	2.95049773	117.745477
225.233111	1.90639674	3.33449463	107.329452
228.421776	1.87057812	2.96861776	105.892253
243.01845	1.83103418	2.96221407	99.5099627
249.477327	1.88240882	2.91134987	98.2316292
263.418696	1.90163948	2.93438484	93.0507106
285.633692	1.97929866	3.20047128	85.9414003
287.856909	1.88492041	2.86652492	85.8899272
292.712885	1.85466977	2.6978884	84.912697
300.477411	1.89351582	2.67740833	83.0602773
313.840519	1.89672577	2.65922732	79.4092317
310.8078	1.86468413	2.42863878	81.0833696
321.232072	1.85498209	2.4108844	77.6549641
314.4151	1.80269017	2.16417479	79.2862474
316.517473	1.78742292	2.05951497	78.6042134
321.381984	1.75507736	2.03051767	77.5070534

II. USING THE STOPPING DISTRIBUTION

Here I develop some general calculations for using the stopping distribution. The first is to calculate a field distribution in a nonuniform field situation. A particularly simple (yet interesting) instance of this is the Meissner phase of a superconductor.

For a superconductor in the Meissner Phase, the magnetic field falls as $B_0 e^{-\alpha z}$ away from the surface, where $\alpha = 1/\lambda$. First let's assume a completely uniform stopping distribution for ^{8}Li, i.e. the probability density of finding ^{8}Li at depth z ($\mathcal{P}(z)$) is just $1/d$ up to the maximum implantation depth d. We will see how to relax this assumption in a moment. First, what should the field distribution function ($P(B)$) look like qualitatively? The maximum field is clearly B_0 and the minimum is $B_0 e^{-\alpha d}$. Many more z values correspond to fields near the minimum field, so we expect $P(B)$ to be a maximum

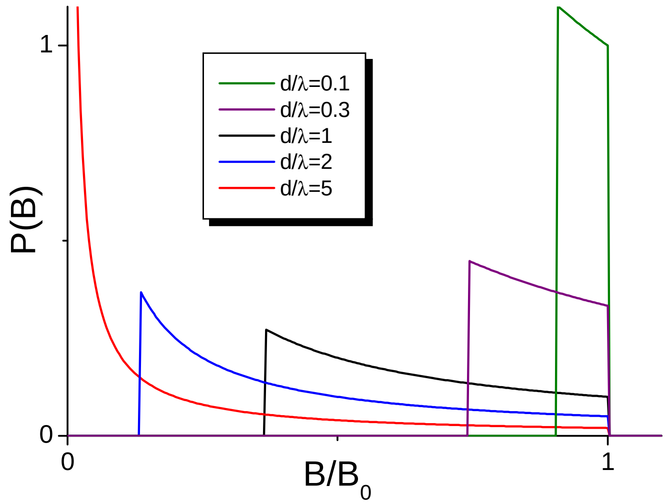

FIG. 4: The field distributions for a uniformly distributed probe in the Meissner state of a superconductor in a magnetic field B_0 smaller than the critical fields for a range of ratios of the maximum implantation depth relative d relative to the penetration depth λ.

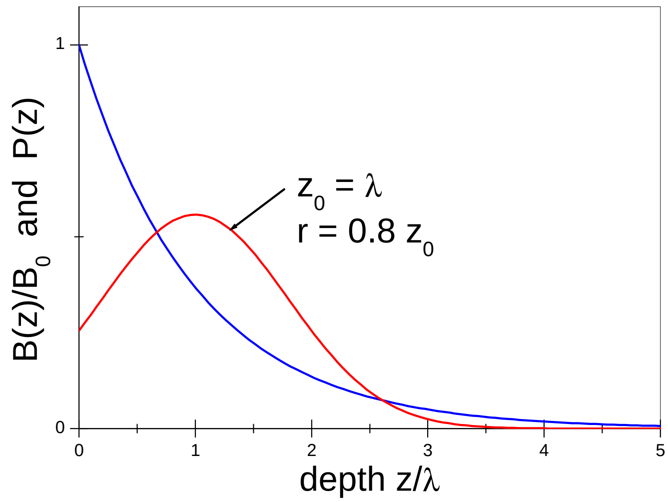

FIG. 5: An example of the (truncated) gaussian stopping distribution (properly normalized) to the normalized magnetic field profile.

there. One can calculate $P(B)$ in the following way[8]:

$$P(B) = N \int_0^\infty \mathcal{P}(z) dz \delta(B - B(z)) \quad (2)$$

$$= \frac{N}{d} \int_0^d dz \delta(B - B(z)), \quad (3)$$

where N is a factor ensuring normalization of $P(B)$. Using the well-known property of the Dirac delta function:

$$\delta(f(z)) = \sum_i \frac{\delta(z - z_i)}{\left|\frac{df}{dz}\right|_{z_i}}, \quad (4)$$

where z_i are the i distinct zeros of f, we get

$$P(B) = \frac{N}{d} \int_0^d dz \frac{\delta(z - z_1)}{| - \alpha B_0 e^{-\alpha z_1}|}, \quad (5)$$

where $z_1 = -\lambda \ln(B/B_0)$ is the only zero of δ's argument. From this,

$$P(B) = \begin{cases} \frac{N}{d\alpha B} & \text{for } z_1 \in [0, d] \\ 0 & \text{elsewhere,} \end{cases} \quad (6)$$

or equivalently,

$$P(B) = \begin{cases} \frac{N}{d\alpha B} & \text{for } B \in [B_0 e^{-\alpha d}, B_0] \\ 0 & \text{elsewhere.} \end{cases} \quad (7)$$

One can use the normalization condition, $\int P(B) dB = 1$ to find that $N = 1$. Fig. 4 shows $P(B)$ for variety of d/λ values. Clearly from the form of $P(B)$ if the implantation depth is infinite, P(B) becomes infinitely peaked at $B = 0$.

Lets try a more realistic ^{8}Li stopping distribution $\mathcal{P}(z)$ like a gaussian,

$$\mathcal{P}(z) = A \exp(-(z - z_0)^2/2r^2), \quad (8)$$

where A is a normalization factor, z_0 is the most probable stopping depth and r is a measure of the range straggling. Fig. 5 shows an example of this stopping distribution together with the spatial dependence of the magnetic field. Now we can proceed to calculate the field distribution.

$$P(B) = N \int_0^\infty \mathcal{P}(z) dz \delta(B - B(z)) \quad (9)$$

$$= NA \int_0^\infty dz e^{-\frac{(z-z_0)^2}{2r^2}} \delta(B - B(z)) \quad (10)$$

$$= NA \int_0^\infty dz e^{-\frac{(z-z_0)^2}{2r^2}} \frac{\delta(z - z_1)}{| - \alpha B_0 e^{-\alpha z_1}|} \quad (11)$$

$$= NA \frac{e^{-\frac{(\lambda \ln(B/B_0) + z_0)^2}{2r^2}}}{\alpha B}, \quad (12)$$

for $B \in (0, B_0]$. Note A has units of 1/length, so P has units of 1/field and N is unitless. Note that as $B \to 0$, the singular behaviour (for $d \to \infty$) we had with the uniform stopping distribution is now cut off by the gaussian in the numerator, and we can take the integral to $z \to \infty$.

For the sake of plotting this distribution, let's assume that the straggling $r = 0.8 z_0$ (typical). Fig. 6 shows the resulting distribution $P(B)$ for a range of values of z_0/λ. To compare this with Fig. 4, use $z_0 \approx d/2$. Note there is still a sharp cutoff in $P(B)$ at the high field side, corresponding to the finite value of $\mathcal{P}(z)$ at the surface, i.e. the depth of maximal field B_0.

This particular example may be relevant for low field studies in superconductors similar to what has been done with LEμSR[9], where B could be the static field **or** the RF field B_1. For the LE muons, the stopping distribution was

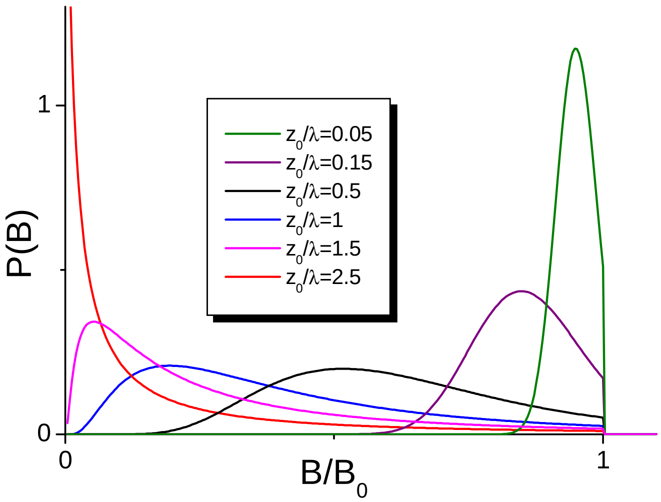

FIG. 6: The field distributions for a gaussian distributed probe in the Meissner state of a superconductor in a magnetic field B_0 smaller than the critical fields for a range of ratios of the maximum of $\mathcal{P}(z)$, the most probable implantation depth, z_0 relative to the penetration depth λ. The range straggling r is a fixed fraction 0.8 of z_0.

taken directly from TRIM.SP without parametrization, see Fig. 2 of Ref.[9] and note the absence of scatter. This approach is certainly more general purpose than trying to parametrize the results of TRIM.SP. But either way, we rely on the correctness of the monte carlo simulations. I hope this introduction helps us to focus on the relevance of the stopping distribution and motivates progress in this direction.

[1] e.g. see the textbook: *Ion Implantation, Sputtering and their Applications* by P.D. Townsend, J.C. Kelly and N.E.W. Hartley (Academic, NY, 1976).
[2] *Ion Implantation Science and Technology* J.F. Ziegler ed. (Academic, NY, 1988).
[3] http://www.srim.org/
[4] E. Morenzoni *et al.*, NIMB **192**, 254 (2002).
[5] P.C. Gregory, book on Bayesian Statistics, used for Phys509 at UBC.
[6] D.L. da Silva *et al.* NIMB **175-177**, 98 (2001).
[7] T.R. Beals *et al.* Physica B **326**, 205 (2003).
[8] There are other ways to do this, see the "Density of Levels" discussion in Chapter 8 of Ashcroft and Mermin.
[9] T.J. Jackson *et al.*, Phys. Rev. Lett. **84**, 4958-4961 (2000).