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Radiation transport calculations for the new ion beam laboratory at Sandia National Laboratory

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A new Ion Beam Laboratory (IBL) is currently under construction at Sandia National Laboratory in Albuquerque, NM, USA. Three existing accelerators will be moved to the IBL, and two more will be purchased to replace existing systems. The IBL will have extensive radiation shielding that will enable a number of new experiments that will be discussed in this paper. This paper also provides the details of extensive radiation transport calculations that were used to determine the thickness and height of the shield walls.

Keywords: Ion-photon emission microscopy; ion beam analysis; ion-luminescence; phosphors; micro-fabrication; proton beam lithography; radiation transport; radiation shielding.

Un Laboratorio de gases iónicos (IBL por sus siglas en inglés, Ion Beam Laboratory) se está construyendo actualmente en el Laboratorio Nacional Sandia en Albuquerque, Nuevo México, USA. Tres aceleradores existentes se moverán al IBL y dos más serán adquiridos para reemplazarlos. El IBL tendrá una extensa protección contra la radiación que permitirá realizar muchos experimentos nuevos que se discuten en este artículo. Este artículo también provee detalles sobre los cálculos exhaustivos relacionados con el transporte radioactivo que se emplearon para determinar el grueso y la altura de las vallas/paredes protectoras.

Descriptores: Microscopía por emisión de ion-fotón; análisis con haces de iones; luminiscencia iónica; fosforos; micro-fabricación; litografía por haz de protones; transporte y blindaje de radiación.

1. Introduction

Sandia National Laboratories in Albuquerque, NM (SNL/NM) is in the process of replacing a 50+ year old accelerator building with a new Ion Beam Laboratory (IBL) facility. The IBL facility will be a unique stand alone capability within the Department of Energy/National Nuclear Security Administration (DOE/NNSA) that employs accelerated ions for a breadth of activities within both the DOE and NNSA. These activities range from applications in support of materials science studies of radiation effects, materials aging and performance. The IBL is currently performing scientific measurements critical to microscopic diagnostics of radiation sensitivity of integrated circuits (ICs), and calibrations of critical radiation detector systems not performed anywhere else in the NNSA complex.

Further, work in this facility supports scientific studies of materials properties performed for both science and engineering projects. The accelerators in the IBL facility are used routinely to perform composition-depth analysis (high-energy accelerators) and materials modification (low-energy ion implanters). Examples are numerous and include: the study and prediction of corrosion behavior of materials, measurements of H isotope concentrations retained in tokamak first walls, and the development of super-hard thin metal films. These capabilities have permitted Sandia to deepen its understanding of material processes involving a rich variety of scientific and engineering disciplines in a manner that could not be accomplished otherwise.

The equipment in the current IBL will be relocated to the new building except two of the older accelerators that will be replaced with new commercially-available instruments to greatly improve our ability to develop, analyze and evaluate micro- and nanotechnologies for future applications within DOE and NNSA. As such, the new IBL facility will provide a state-of-the-art environment for performing ion beam irradiations for applications that directly impact these programs, balanced with fundamental research into radiation effects and materials science.

In this paper, we

1) outline some of the current programs being carried out in the existing IBL,

2) describe the new IBL placing emphasis on the shielding design, and

3) discuss the new science that will be enabled by both the new equipment and shielding provided by the new building.

2. Accelerators

The Ion Beam Laboratory (IBL) facility is an accelerator laboratory totally unlike any other such lab in the DOE/NNSA complex. The five accelerators that will make up the IBL facility will be used exclusively in the areas of condensed matter physics, materials science, nanotechnology and radiation effects science, instead of being applied to the study
of elementary particles, nuclear or atomic physics. This section summarizes the capabilities and some of the programs for both the existing accelerator systems and those to be purchased with the new IBL building.

The accelerator systems that will be located in the new IBL are shown schematically in Fig. 1, together with their energy range and current or envisioned application areas.

- **Tandem + RFQ Linac (1.9 – 400 MeV).** This unique system [1] uses the HVEC EN Tandem Pelletron to inject heavy ions into an AccSys Radio Frequency Quadrupole (RFQ). When the ions exit, they have an energy/mass of 1.9 MeV/amu. For Bi ions, this is an energy of 400 MeV. Radiation Effects Microscope (REM) [2] is the technique exclusively performed on this system to pinpoint the Single Event Effect (SEE) problems in integrated circuits [3]. The accelerated high energy heavy ions simulate outer space cosmic rays that can plague the performance of ICs used in satellites and other instruments.

- **Tandem (0.5-50 MeV).** The tandem is a Van de Graaff style electrostatic accelerator that has been retrofitted with Pelletron chains. There are 4 negative ion sources and 10 beamlines associated with the tandem accelerator. In addition to standard applied nuclear physics materials analysis or Ion Beam Analysis (IBA) techniques, such as RBS, ERD, NRA, and PIXE, the Tandem is also used to generate highly localized fields of particle irradiation for REM [4]. There are 4 nuclear microscopes located on the Tandem.

- **New Pelletron (0.3-3 MeV, replacing existing AN Van de Graaff Accelerator).** In addition to traditional IBA, the new Pelletron will provide beams of high energy deuterons into the High Radiation Room where selected nuclear reactions will be used to profile the concentration of various light isotopes in depth. This capability was lost ~15 years ago at Sandia, when the operation at another accelerator building was terminated. There will also be a new nuclear microprobe added to this accelerator for performing micro PIXE and potentially Proton Beam Writing (PBW) [5]. The replacement accelerator is to have exceptional energy definition, enabling nuclear microscopy experiments with beams 10 times smaller than the 1 micron size spots currently available.

- **Implanter (10-350 keV).** This accelerator will be the last remaining research ion implantation system at Sandia. It was instrumental in developing the n- and p-type doping of both Si and compound semiconductor devices. This implanter has been used as a highly controlled method of introducing atoms such as Cl into metals that can lead to corrosion. We are one of the few groups in corrosion science that can test corrosion mechanisms by selective ion-beam modification of materials [6]. A NanoBeam has also been developed on this implanter for purposes of performing single dopant atom implants into Si-based quantum computers [7].

- **New NanoImplanter (10-100 keV, replacing the existing Eaton Implanter).** The NanoImplanter will be capable of providing nanometer diameter beams for implantation and atomic-level modification of components important to future research at Sandia involving micro and nanotechnology. This system is much like a conventional Focused Ion Beam (FIB) system except that eutectic alloy liquid metal sources coupled with a Wien mass filter will permit the selection of a rich variety of ions to be accelerated to energies up to 100 keV. The focal spot of this system will be in the 10 nm range. Because of the variety of ions, the high energy, and 10 nm spot size, the system will be unique in both North and South America.

- **Pulsed Laser Deposition (PLD, 1-100 eV).** The PLD system has been used to make samples for evaluating the performance limits and mechanisms that give rise to high-strength metals. This research supports work by engineers at Sandia who develop processes to produce ultrafine-grain metal structures with high strength for micromachining applications.
There are heavily radiation shielded areas for all three accelerators, and two of the experimental areas. For example, the Pelletron Room has a small target area in which external micro PIXE can be performed with a focused beam extracted from the vacuum system. But the main shielded area for performing experiments is that labeled “High Rad” in the figure. This area was designed so that experiments could be performed in this room that produce up to 5 rem/hr of neutrons and 2.5 rem/hr of high energy gamma radiation. Personnel radiation safety is paramount at Sandia as it is in all the DOE/NNSA Laboratories, and so it was critical that the thickness, height and cement density be adequate to protect the staff of the IBL from being exposed to the radiation produced in the High Radiation Room (HRR). The next section outlines the calculations used to determine these parameters.

3.2. Radiation shielding and environmental impact calculations

3.2.1. Within the IBL

We have employed two independent widely used codes, MCNPX [8] and SCALE [9], to evaluate the doses inside and outside the IBL, corresponding to different shielding designs. The two codes’ results usually agree within the 20%. Table I shows the “Source Terms”, indicating the activities of the two most powerful sources in the High Radiation Room (HRR), named SI-1 (neutrons) and SI-2 (gammas) (positioned at the endstations labeled “n-det calibration” and “NRA”) respectively in Fig. 2. For SI-1 two neutron energies have been considered: 2.5 and 14 MeV. The “power” of a source is customarily described by the dose at a distance of 30 cm.

From the Source Term one calculates the Dose Rate at the points of interest. In particular, in case of the code MCNPX, the applicable formulas are:

\[
\text{SourceTerm}[Bq] = \frac{1}{\text{RF}}[Bq \cdot cm^{-2}/(rem \cdot h^{-1})] \\
\times \text{DoseRate}[rem \cdot h^{-1}] \cdot \frac{4\pi \cdot r^2}{[cm^2]} \\
\text{DoseRate}(r)\left[\frac{rem \cdot h^{-1}}{Bq}\right] \cdot \text{SourceTerm}[Bq]
\]

The “Response Factor” RF is a coefficient that transforms the Particle-Flux[#radiation-particles/(cm²·s)] into the Dose-Rate[rem·h⁻¹]. The units of the two quantities are chosen according to an established tradition. \( P(r) \), used by MCNPX in \( [rem \cdot h^{-1}/Bq] \) unit, is the average fluence per hour that a single particle (either n or \( \gamma \)) generates at the position \( r \). Using the formulas above, we have evaluated the DoseRate\((r)\) at many points \( r_i \) for different thicknesses of the walls. Table II shows the Dose Rate in several key points \( r_i \) of the new IBL, as described in the Fig. 2. Numbers refer to the wall’s thicknesses that have been finally chosen, i.e. 18”, 24”, and 30” (only for the HRR).

<table>
<thead>
<tr>
<th>Sources Name</th>
<th>SI-1</th>
<th>SI-1</th>
<th>SI-2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle</td>
<td>neutrons</td>
<td>neutrons</td>
<td>gammas</td>
</tr>
<tr>
<td>Energy (MeV)</td>
<td>2.5</td>
<td>14</td>
<td>3</td>
</tr>
<tr>
<td>Dose Rate @ 30 cm (rem·h⁻¹)</td>
<td>5</td>
<td>5</td>
<td>2.5</td>
</tr>
<tr>
<td>RF=Response Factor</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(rem·h⁻¹)/(cm²·Bq)</td>
<td>1.28E-04</td>
<td>1.95E-4</td>
<td>3.96E-06</td>
</tr>
<tr>
<td>A=Source Activity (Bq)</td>
<td>4.42E+08</td>
<td>2.91E+8</td>
<td>7.14E+09</td>
</tr>
</tbody>
</table>

Table I. Description of the two main sources present in the High Radiation Room or HRR. The Response Factor, converting the Particle-Flux [#radiation-particles/(cm²·s)] into the Dose-Rate (Rem/h) depends on the neutron or gamma energy. We follow the energy subdivision by Straker-Morrison [10]. Values have been obtained with the SCALE (2005) code.
Prompt or direct radiation and a possible emission of radioactive effluents from accelerator operation may have an off-site environmental impact. Air-born, ground and surface water contamination may become a risk only in facilities for the production of radio-isotopes or exotic beams. Here we only describe the prompt or direct radiation that affects the area around the source within hundred of meters and has to be taken into account in the design of the facility. This off-site radiation is usually referred to as ‘skyshine’, because, in most cases, while sufficient shielding is provided in the horizontal direction (by thick concrete walls), the roof shielding has to be kept limited to contain the costs. This results in more radiation (essentially neutrons) that is emitted vertically being scattered back to ground level. For a more complete review of the radiation at long distances see Moritz [11]. Neutron skyshine coming from the high radiation room (HRR) of the IBL is the predominant exposure pathway to persons outside the IBL building. The annual dose projected to be received by IBL staff at various positions in the new IBL. While not shown, these results agree with SCALE calculations within 20%

### Table II. Dose rates calculated using MCNPx to be received by IBL staff at various positions in the new IBL. While not shown, these results agree with SCALE calculations within 20%

<table>
<thead>
<tr>
<th>Detectors</th>
<th>x cm</th>
<th>y cm</th>
<th>Mnpx-nn rem·h⁻¹/Bq</th>
<th>Mnpx-nγ γ-DoseR mrem·h⁻¹</th>
<th>Mnpx-nγ γ-DoseR mrem·h⁻¹</th>
<th>SI-1(n 14MeV)(3004.-241)</th>
<th>SI1yoγg.0MeVpozz8ysyx4p</th>
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</thead>
<tbody>
<tr>
<td>DQ</td>
<td>4073</td>
<td>-172</td>
<td>4.4E-13</td>
<td>1.3E-01</td>
<td>2.1E-14</td>
<td>6.1E-03</td>
<td>2.5E-15</td>
</tr>
<tr>
<td>DE</td>
<td>1442</td>
<td>-142</td>
<td>7.1E-14</td>
<td>2.1E-02</td>
<td>2.7E-15</td>
<td>7.8E-04</td>
<td>1.3E-16</td>
</tr>
<tr>
<td>DG</td>
<td>2478</td>
<td>-2633</td>
<td>6.4E-14</td>
<td>1.9E-02</td>
<td>1.7E-15</td>
<td>4.9E-04</td>
<td>1.8E-16</td>
</tr>
<tr>
<td>DH</td>
<td>1406</td>
<td>-2816</td>
<td>5.5E-14</td>
<td>1.6E-02</td>
<td>1.4E-15</td>
<td>4.0E-04</td>
<td>1.8E-16</td>
</tr>
<tr>
<td>DT</td>
<td>5036</td>
<td>-172</td>
<td>1.9E-13</td>
<td>5.6E-02</td>
<td>7.4E-15</td>
<td>2.1E-03</td>
<td>9.6E-16</td>
</tr>
<tr>
<td>DU</td>
<td>1173</td>
<td>-139</td>
<td>8.3E-14</td>
<td>2.4E-02</td>
<td>2.6E-15</td>
<td>7.5E-04</td>
<td>1.7E-16</td>
</tr>
<tr>
<td>Door3</td>
<td>2325</td>
<td>-421</td>
<td>2.9E-13</td>
<td>8.5E-02</td>
<td>1.8E-14</td>
<td>5.1E-03</td>
<td>9.5E-16</td>
</tr>
<tr>
<td>Door4</td>
<td>2402</td>
<td>-683</td>
<td>1.7E-13</td>
<td>4.8E-02</td>
<td>5.3E-15</td>
<td>1.5E-03</td>
<td>6.7E-16</td>
</tr>
<tr>
<td>Door5</td>
<td>1533</td>
<td>-754</td>
<td>2.7E-13</td>
<td>7.8E-02</td>
<td>1.3E-14</td>
<td>3.8E-03</td>
<td>8.3E-16</td>
</tr>
<tr>
<td>DA</td>
<td>3847</td>
<td>1370</td>
<td>1.7E-13</td>
<td>4.8E-02</td>
<td>5.2E-15</td>
<td>1.5E-03</td>
<td>6.7E-16</td>
</tr>
<tr>
<td>DC</td>
<td>2470</td>
<td>1260</td>
<td>4.7E-14</td>
<td>1.4E-02</td>
<td>1.5E-15</td>
<td>4.4E-04</td>
<td>2.1E-17</td>
</tr>
<tr>
<td>DI</td>
<td>3146</td>
<td>-3446</td>
<td>4.8E-14</td>
<td>1.4E-02</td>
<td>1.2E-15</td>
<td>3.4E-04</td>
<td>1.5E-16</td>
</tr>
</tbody>
</table>

The same doses may approximately be calculated by using the Stapleton et al. formula [12] that comes from basic nuclear physics considerations as described in the following. As the threshold of neutron induced nuclear reactions with the air elements (N, O, Ar) lies near or above 20 MeV, the interactions below this energy are restricted to elastic scattering. The high energy nuclear interaction lengths for $N_2$ and $O_2$ are of the order of 750 m in the case of air (density=1.2·10⁻³ g·cm⁻³) and hence the high energy neutrons effectively escape to great distances. Because only low energy neutrons can be scattered into the backward direction, near the source only these neutrons are important, while at distances comparable to the nuclear interaction length, the high energy neutrons will predominate. The neutrons, lighter than the air nitrogen and oxygen nuclei, lose their energy only after many elastic scatters, and the primary reduction in fluence out to a few hundred meters mainly derives from geometrical factors. As particle number must be conserved, the dose at distance $r$ from the source, is inversely proportional to the area over which the particles are dispersed ($\sim 1/r^2$). There is also an attenuation that is expressed by an exponential factor and becomes important at distances of several hundreds of meters. Stapleton et al. [12] carried out a complete analysis, used the “importance functions” calculated by Alsmiller et al. [13], and took into account the spectrum of neutrons and how this is modified by the scattering off the air and even the ground (since the high energy neutrons survive to a greater distances). Their expression for the dose $H(r)$ per “skyshine
neutron” as function of the distance \( r \) from the source is:

\[
H(r) = \frac{a}{(r + b)^2} e^{-\frac{r}{\lambda}}
\]

where, \( E_c \) (“cutoff energy”) is the highest energy of a given neutron spectrum. A best fit to this formula offered the values for \( a, b \) and \( \lambda \) listed in Table III. In this method, if the source is known only in terms of the equivalent dose, then it must first be converted to neutrons using the \( g \) factors of the last column of the Table. These factors are the averaged equivalent dose over the composite spectrum with cut-off energy \( E_c \).

### 3.3. High radiation experiments

As indicated above, it has been 15 years since moderately high radiation experiments could be performed using the IBL accelerators. Not surprisingly, some of the first envisioned to be performed in the new IBL involve the \((d,p)\) reactions [15] using the new Pelletron for profiling light isotopes in solids, as this was the main capability that involved high radiation that was lost.

But in addition, we foresee many other new measurements that will be performed in the High Radiation Room (HRR), which are enabled by its significant shielding. \((p,\gamma)\) experiments with proton beams of energies up to the 12 MeV maximum provided by the Tandem will now be capable of being performed. In this chamber we also expect to use proton exposures above \((p,\gamma)\) thresholds to perform Charged Particle Activation Analysis (CPAA) [16], to measure wear on components critical to National Defense and advanced energy initiatives.

There are even high radiation experiments we plan that involve the Implanter. These will involve the generation of 14 MeV neutrons using the \(T(d,n)\) nuclear reaction. A special type of Elastic Recoil Detection (ERD) will be performed in air to profile all three Hydrogen isotopes. The main advantage of this type of ERD is that components can then be analyzed that are unsuitable for normal vacuum analysis because of size or radioactivity [17]. With this technique the 14 MeV neutrons pass through the backside of the sample, and when the exit from the front surface (the near surface region to be analyzed), they recoil H isotopes from the sample into special ion energy-mass detectors called particle telescopes. Many applications for using this technique have been envisioned from national security to fusion energy research to studies of importance to national heritage.

### 4. Summary

The impact made possible by the unique combination of accelerators in the IBL facility stems from the fact that virtually any isotope can be accelerated to energies ranging from 1 eV to almost 400,000,000 eV (see Fig. 1. The lowest energy ions (PLD) are used primarily to grow new materials and to produce tailored nanostructures; medium energy ions from two more accelerators (Nanobeam and Implanter) modify the composition and properties of the near-surface region of solids. The high energy ions (Pelletron, Tandem and RFQ accelerators) are used to perform a wide array of applied nuclear physics techniques to determine isotopic composition or to provide ions for microscopically assessing radiation effects in electro-optical-mechanical devices.
Perhaps the three most important new aspects of the new building are
1) the radiation shielding,
2) the NanoImplanter, and
3) the fact that the new IBL will be in an unclassified area.

The radiation shielding will allow experiments we could never have performed in the current building, and this will open entirely new avenues of research and development to be performed in the IBL. As indicated above, the NanoImplanter will be unique in the USA, and is expected to find critical applications in the area of nanoscience and nanotechnology. But for most of the attendees of this Symposium on Radiation Physics, the third aspect may be the most important, because by being outside of the classified security area at Sandia, interactions and collaborations between Sandia staff and Mexican or other foreign scientists will be much easier.

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