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Abstract

We have studied the structural damage of W-Re targets produced by electrons with energies of several GeV and under different conditions of total number of electrons, beam shape and target depth. We report the differences in damage levels for different designs considered in the construction of the next generation of linear accelerators, and discuss the possible effects in the lifetime of these targets. Due to the complexity of the problem, which requires following the trajectory of GeV electrons down to eV energies, this work utilized different simulation tools, from Monte Carlo codes of hadronic and electromagnetic interactions such as FLUKA, to molecular dynamics simulations of defect production. Our work shows that the final defect production depends not only on

the total number of electrons and energy, but also on the geometry of the target. Combining different values of energies and target geometry could be a way of reducing the maximum damage in these systems.

I. Introduction

Radiation damage due to electron irradiation has not been considered so far as a limiting step in the development of targets for linear accelerators. However, as higher doses are reached, understanding the total damage produced in these targets becomes increasingly critical in order to predict their lifetime. Such is the case of the Next Linear Collider, NLC [1], where doses are expected to reach more than one order of magnitude larger values than in current and previous generations of linear accelerators. Targets used in the Stanford Linear Collider [2] (SLC) provide a source of evidence for the damage accumulated in Tungsten-Rhenium (W-Re) targets.

W-26% Re alloys were selected as SLC target materials because of their exceptional physical properties such as high strength and ductility at the anticipated target operating temperatures, between 115 and 200°C [3]. At 150°C, ductility of these alloys increases to 10% with no significant decrease in yield strength, maintaining it at 1100 MPa [4]. Not anticipated were the catastrophic changes in mechanical properties of these materials due to irradiation, which lead to target failure [3], although the detrimental effects of irradiation of materials are well documented by the fusion and fission communities [5, 6, 7]. In particular, an effect of concern for body centered cubic (BCC) materials is the increase in the ductile to brittle transition temperature (DBTT) with increasing irradiation dose. Shifts in the value of DBTT have been observed in W alloys after neutron irradiation [8]. Some of these studies show a detrimental effect of Re in the temperature shift during irradiation, possibly due to formation of Re-rich sigma and chi precipitates [9, 10]. Models that predict the performance of these targets under different conditions of energy of the electrons, total dose, beam size and target size are necessary in order to design targets for future accelerators. In this paper we make a first attempt to model the structural damage produced by GeV electrons when interacting with tungsten-based targets.

Several steps are necessary to be able to predict the total damage in these targets. Models of the interaction of electrons with different targets have been extensively used by the high-energy physics community for many decades to understand the production and multiplication of electrons in the target. However not much attention has been devoted to the study of the defect produced damage in the target. These codes follow the production of energetic recoils from electron interactions and therefore can be used to calculate the point defect production from these recoils as a function of the energy transfer, as well as from spallation products and neutrons. The first step in this study was to store the three-dimensional (3D) distribution of recoils from spallation reactions, neutrons and fission products, as well as their energy as calculated by FLUKA [11]. This is explained in the second section of this paper. In a second step, this data was used to calculate the defect distribution in the target, as explained in Section III. A linear accumulation of damage is assumed in order to calculate the final dose for different configurations. This data is presented in Section IV. Finally, we discuss the validity of the approximations done in this study and how to extrapolate this data to obtain the lifetime of these materials.

II. FLUKA calculations

The 3D distribution of energetic products of the electron – target interaction was stored from the FLUKA [11] calculations. Four different products are generated by the interaction of the electrons with the target that can induce structural damage in the material: recoils from spallation reactions, light fragments, fission products and neutrons. The position (x, y, z) and the energies are saved for all energetic events and for a large number of incident electrons, in order to get a statistically significant distribution. In the cases reported here a total of $5x10^5$ events were simulated. All the results presented are obtained from an average over these events. The initial electron beam is approximated with a Gaussian distribution.

We have simulated high-energy electron irradiation damage in four different targets. The characteristics of each target are shown in Table I;one target is representative of those used at the SLC accelerator in Stanford, another is representative of an advanced accelerator such as the NLC and two test other targets. These last two targets we note Test Target 1 and Test Target 2. Test Target 2 has the same characteristics as the NLC target except for the energy of the electrons, and it will be used in these calculations to study the effect of the energy in the final defect production. Test Target 1 is designed for a short irradiation time, and as a possible experiment to be performed in the future that can be used as a validation of the calculations presented here.

Figure 1 shows the recoil distribution as obtained from FLUKA for the case of the NLC target. Figure 1(a) shows the radial distribution, where zero is the center of the beam. Figure 1(b) shows the recoil as a function of depth of the target. Notice in this case that the number of recoils increases with depth, as expected, due to the cascade effects of the electrons.

III. Defect production

Using the 3D distribution and energy of the recoils for spallation reactions, neutrons and fission products obtained by FLUKA we calculate the total number of defects produced in the target. In order to do this calculation we use the modified Kinchin-Pease model [12]. According to this model the number of defects (vacancy-interstitial pairs) produced (N_D) by energetic recoils in a target is:

$N_D = 0.8 * E_D / (2*E_{th})$ where E_D is the damage energy, or energy deposited into elastic collisions (the energy calculated in FLUKA) and E_{th} is the threshold energy, or minimum energy to produce a defect in the target. For the case of tungsten, the threshold displacement energy used in these calculations is 90eV.

Some corrections must be applied to the Kinchin-Pease model. Molecular dynamics simulations performed during the last decade [13, 14, 15] have shown that the Kinchin-Pease model overestimates the total number of defects produced at energies above a few keV. The reason for this discrepancy is the assumption of a binary collision model in the Kinchin-Pease model. Molecular dynamics [16] has shown that multiple collision events play a significant role in the final number of defects produced. We have used molecular dynamics simulations to study the number of defects produced in tungsten for different energies, from 1 to 100 keV. Figure 2 shows the defect efficiency (η), or the ratio between the number of defects obtained from molecular dynamics and those predicted by the Kinchin-Pease model. This defect efficiency reaches a constant value of 0.2 for energies larger than 10keV. It is interesting to point out that this value of 0.2 seems to be independent of the material studied. Copper and iron seem to reach the same value of 0.2 [14, 15].

Thus, in our calculations of the total number of defects we have corrected the Kinchin-Pease model by the factor obtained in this molecular dynamics calculation. From the MD defect production curve in Figure 2 we obtain the following function:

For $E_D < 3$ keV

$$\eta = 0.00506 * E_D \text{ (in keV)} + 1.0184 * E_D^{-0.667} \text{(in keV)}$$

and for $E_D > 3$ keV,

$$\eta = 0.2$$

The energies calculated with molecular dynamics are only up to 100keV, while the energies obtained from FLUKA are much higher. However, our molecular dynamics simulations also show that at energies above 30 keV, cascades break into smaller sub-cascades. Therefore, it is possible to simulate the total spectrum of energies using the results of these molecular dynamics simulations. Figure 3 shows the result of such a molecular dynamics calculation. In Figure 3(a) we show the number of defects produced in tungsten by a 30 keV recoil, where a single cascade is generated. The green circles represent vacancies while the red ones represent interstitials. As in previous calculations [13, 14], vacancies are located in the center of the collision cascade with interstitials in the surroundings. No significant clustering of vacancies is observed in these simulations. In Figure 3(b), where the energy of the recoil is 50 keV, clearly two subcascades are formed, with two separate vacancy groups. We should point out that, although the calculations presented here are for pure W, we do not expect significant differences regarding the total number of defects produced since the mass of W and Re are similar.

III.a Spallation and Fission products

For the case of spallation and fissionproducts the above model can be used to calculate the number of defects produced by these energetic atoms. Figure 4 shows a 2D profile of the concentration of defects per electron produced in the SLC target, for the different energetic components. In particular, Figures 4 (b), (c) and (d) show contour plots of the concentration of defects per electron produced by recoils from spallation reactions , by light fragments and by fission products respectively. Colors represent defect levels as a function of target depth and width. Notice that the size of the targets is different for the cases studied, as defined in Table I. The concentration of defects reported here has been obtained as an average over a volume of 0.66 mm x 0.68 mm x 2mm. Colors in the figure represent the defect concentration in defects/cm^3. Observe that the scales change for the different plots in Figure 4. Most of the defects produced are due to spallation products, with concentrations up to 360 defects/cm^3 per incident electron. As expected, light products do not contribute significantly to the total number of defects produced, with defect concentrations four orders of magnitude smaller than for the case of spallation products.

III.b Neutrons

One of the products of the interaction of the electrons with the target is energetic neutrons. A code such as FLUKA provides information about the neutron energy and neutron location. However, in order to extract the defects produced by these neutrons it is necessary to calculate the energy deposited by these neutrons into the lattice in the form of energetic recoils. This can be achieved by coupling this information to a code such as SPECTER [17], which is commonly used by the fusion and fission communities. SPECTER contains libraries of cross sections for displacements for various compounds. Given a neutron energy spectrum this code calculates the total number of defects produced as well as the recoil energy spectrum. We have used SPECTER to calculate recoil spectra for the different energies of the neutrons produced by the electron irradiation and obtained from FLUKA. We have tabulated the spectra as a function of neutron energy and used the energies of these recoils to calculate the final defect production. As above, the defects are obtained from the Kinchin-Pease model combined with the defect efficiency extracted from molecular dynamics. Figure 4(a) shows the concentration of defects per electron due to neutrons produced in a target such as the SLC target.

It is interesting to point out that from all type of reactions produced by the electron-target interactions, neutrons are the ones that produce the largest number of defects, as shown in Figure 4. Defect concentrations can locally reach values up to 10^4 defects/cm^3 per incident electron, two orders of magnitude larger than for the case of recoils.

IV. Total damage and dose effects

We have integrated the number of defects produced per electron due to the different energetic events in order to calculate the total number of defects produced per electron in different conditions. Figure 5(a) shows the total number of defects per electron in the case of SLC. This is the result of adding the defect concentrations in Figure 4. We have also computed the total number of defects per electron expected in the NLC target and in the two other Test Targets. Again, the different target characteristics are provided in Table I.

Figure 5 shows the results of the total defects per electron produced in the four targets considered in this study. From this analysis we obtain that the total number of *defects per electron* is larger in the SLC and Test target 1 cases than in NLC. This difference is just due to the lower energy of the NLC beam with respect to the SLC. The damage per electron due to 30GeV electrons (SLC) is larger than in the case of 6.2 GeV (NLC), approximately 11 times larger.

However, in order to account for the final defect concentration it is necessary to compute the total defect concentration for the total number of incident electrons, since this number is different for the different targets, as shown in the last row of Table I. Figure 6 shows the total number of defects for the total number of electrons for all four targets. The total number of defects is computed simply by multiplying the number of defects (Figure 5) by the total number of electrons (last row in Table I). We express the final damage in terms of dpa, displacements per atom, simply by dividing by the density of the material (in atoms/cm^3). Using this definition we can compare to other irradiation studies of W-Re, since this definition is commonly used to quantify radiation damage effects. The maximum dpa levels obtained from these calculations are below 1 dpa (0.8 dpa maximum for the NLC) for a total time of 3 years, values below those expected in neutron irradiation.

V. Discussion

Table II compares the maximum defect concentrations in all the targets studied. In this table we show the maximum defect concentration as well as the maximum with respect to the SLC target. Notice that the maximum damage in the NLC target is a factor of 1.6 larger than the SLC target. The maximum number of defects per electron in the SLC target is approximately 11 x larger than for the NLC target while the total beam intensity in NLC is ~ 18 times larger than in SLC, which results in this 1.6 higher damage expected in the NLC target. Notice also the different shapes in the damage profile for the NLC and SLC targets as shown in Figures 5 and 6. In the case of the Test Target 1, the maximum damage is slightly smaller than in the SLC target, probably due to the beam size and longer range of the electrons. The beam intensity is also smaller, resulting in a maximum damage ~ 5x smaller than in SLC. Finally, the Test Target 2 configuration results in a much smaller defect per electron due to the low energy (2 GeV), and the final damage is ~ 1.6x smaller than in the SLC target.

An important point must be addressed in this discussion: all the simulations presented above did not include temperature effects. The total number of defects reported here are at room temperature. High temperatures are achieved in the target due to the electron irradiation. Temperature will induce migration of defects and therefore increase recombination between defects. Recombination between vacancy and interstitial type of defects will reduce the total defect concentration. We can, therefore say that the values reported here are an upper limit to the total number of defects expected after irradiation. We should point out that defect diffusion, leading to recombination, clustering and annihilation at larger, extended defects, will also result in solute and impurity transport and could also generate precipitates, detrimental for the mechanical properties of these materials.

VI. Conclusions

To summarize, we have presented a first attempt to quantify the defect densities produced by electron irradiation at GeV energies in W-Re targets for linear accelerators. We have presented results for different target configurations, in particular for the conditions expected in next generation linear colliders such as the NLC. Our simulations show that the number of defects does not increase linearly with energy. For example, SLC and NLC configurations differ by 4.8 times in energy (with SLC having higher energy). However, due to differences in beam size, target geometry, and in the evolution of the electron cascade, the SLC target shows regions with maximum number of defects 11 times larger than in the NLC target (see Figures 5(a) and (b)). That is, the damage per incident electron is more localized in the SLC target. As a result, although the NLC target is expected to have a beam intensity 18 times larger than in the SLC target, the final difference in the total number of defects produced for the total beam intensity is only 1.6 times larger in the NLC target than in the SLC target. A reduction in energy from 6.2 GeV (NLC) to 2 GeV, keeping the beam intensity and the geometry of the sample the same results in a reduction of maximum damage values even below the SLC values, as shown in the example of Test Target 2.

In terms of total defect production, values are below the 1 dpa level for the total time of the target considered and all cases. Neutron irradiated specimens of W-26% Re alloys to levels of 1-2 dpa show that irradiation induced the formation of precipitates that cause both hardening as well as embittlement of the alloy. A reduction of the Re content could reduce the effects of the radiation rembrittlement [10].

Acknowledgements

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Tables

Table I

Characteristics of the target: energy, beam size, electrons per pulse, target depth, frequency, spots in target, total exposure time and total number of electrons in target

	SLC	NLC	Test Target 1	Test Target 2
Energy (GeV)	30	6.2	45	2.0
Beam radius (mm)	0.8	1.6	1.6	1.6
Electrons per pulse	3.5×10^{10}	1.35×10^{12}	2.2×10^{11}	1.35×10^{12}
Thickness (mm)	20.6	13.0	19.0	12.25
Frequency (Hz)	120	120	10	120
Spots in target	60	126	1	126
Total exposure time	3 years	3 years	2 weeks	3 years
Total number of electrons	6.62×10^{18}	1.22×10^{20}	2.66×10^{18}	1.22×10^{20}

Table II

Total damage accumulated for the different targets in DPA (displacements per atom) and normalized to the damage in the SLC target

Target	Energy (GeV)	Max DPA Value	Max DPA Value (Normalized to SLC)
SLC	30.0	0.5	1
NLC	6.2	0.8	1.6xSLC
Test Target 1	45.0	0.1	0.2xSLC
Test Target 2	2.0	0.3	0.6xSLC

Figure Captions:

Figure 1: Recoil distribution from FLUKA for the NLC target (a) from the center of the beam, and (b) as a function of target depth. Observe the increasing number of recoils with target depth.

Figure 2: Damage efficiency as calculated from molecular dynamics and compared to the Kinchin-Pease model for the case of tungsten.

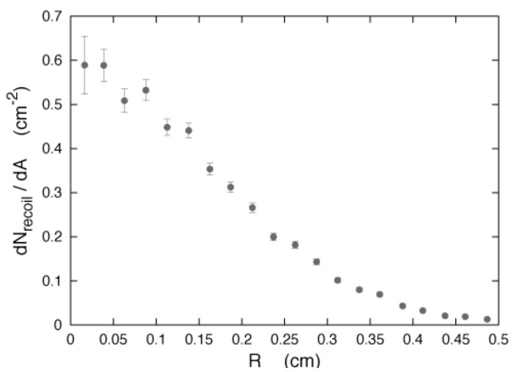
Figure 3: Simulation of defects using molecular dynamics simulations in tungsten due to (a) 30 keV and (b) 50 keV recoils. Green spheres represent vacancies and Red spheres represent interstitials.

Figure 4: Concentration of defects produced in the SLC target per incident electron due to (a) neutrons, (b) recoils from spallation reactions, (c) light fragments and (d) fission products. Damage is calculated in volumes of size 0.66 mm x 0.68 mm x 2mm. Notice the different scales on each figure. Most of the damage produced in the target is due to neutrons.

Figure 5: Total concentration of defects per electron produced in (a) SLC (b) NLC (c) Test Target 1 and (d) Test Target 2. The total number of defects per electron is larger in the SLC and Test target 1 cases than in NLC due to the lower energy of the NLC beam.

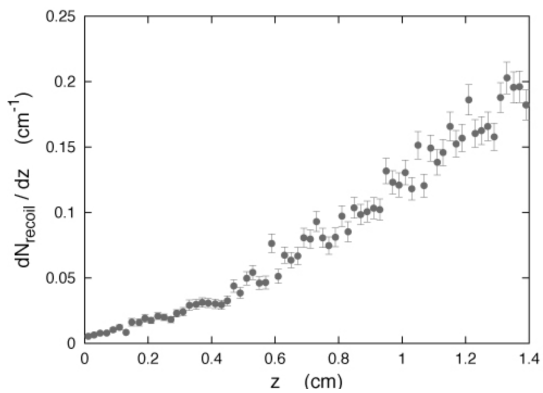
Figure 6: Total concentration of defects for the total beam intensity produced in (a) SLC (b) NLC (c) Test Target 1 and (d) Test Target 2. In this case the beam intensity is given in displacements per atom (dpa). The total number of defects for the total number of electrons is larger in the NLC case than in the SLC and Test targets and the lowest in the Test Target 2 configuration.

Figure 1



0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
dNrecoil / dA (cm-2)
0 0.05 0.1 0.15 0.2 0.25 0.3 0.35 0.4 0.45 0.5
R (cm)

(a)



0.25
0.2
0.15
0.1
0.05
0
dNrecoil / dz (cm-1)
0 0.2 0.4 0.6 0.8 1 1.2 1.4
z (cm)

(b)

Figure 2

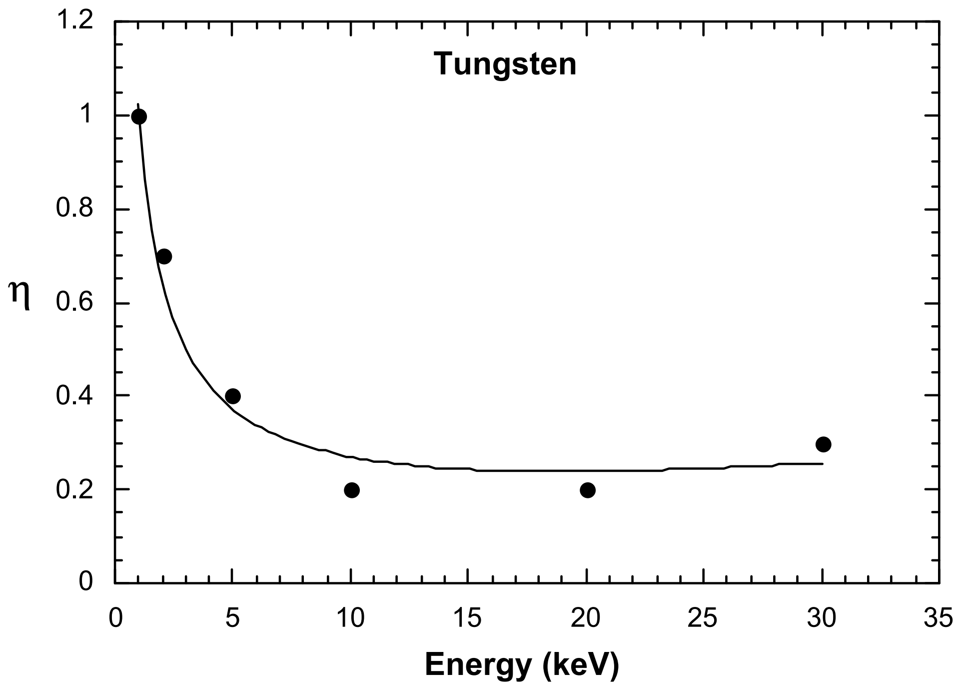
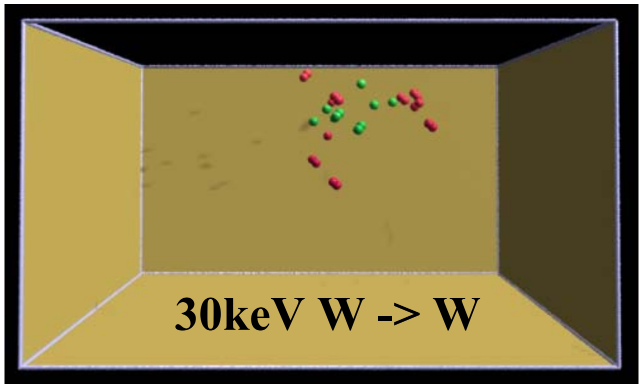
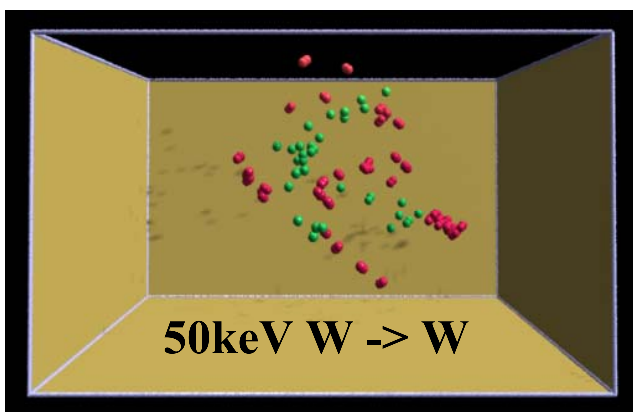


Figure 3



(a)



(b)

Figure 4

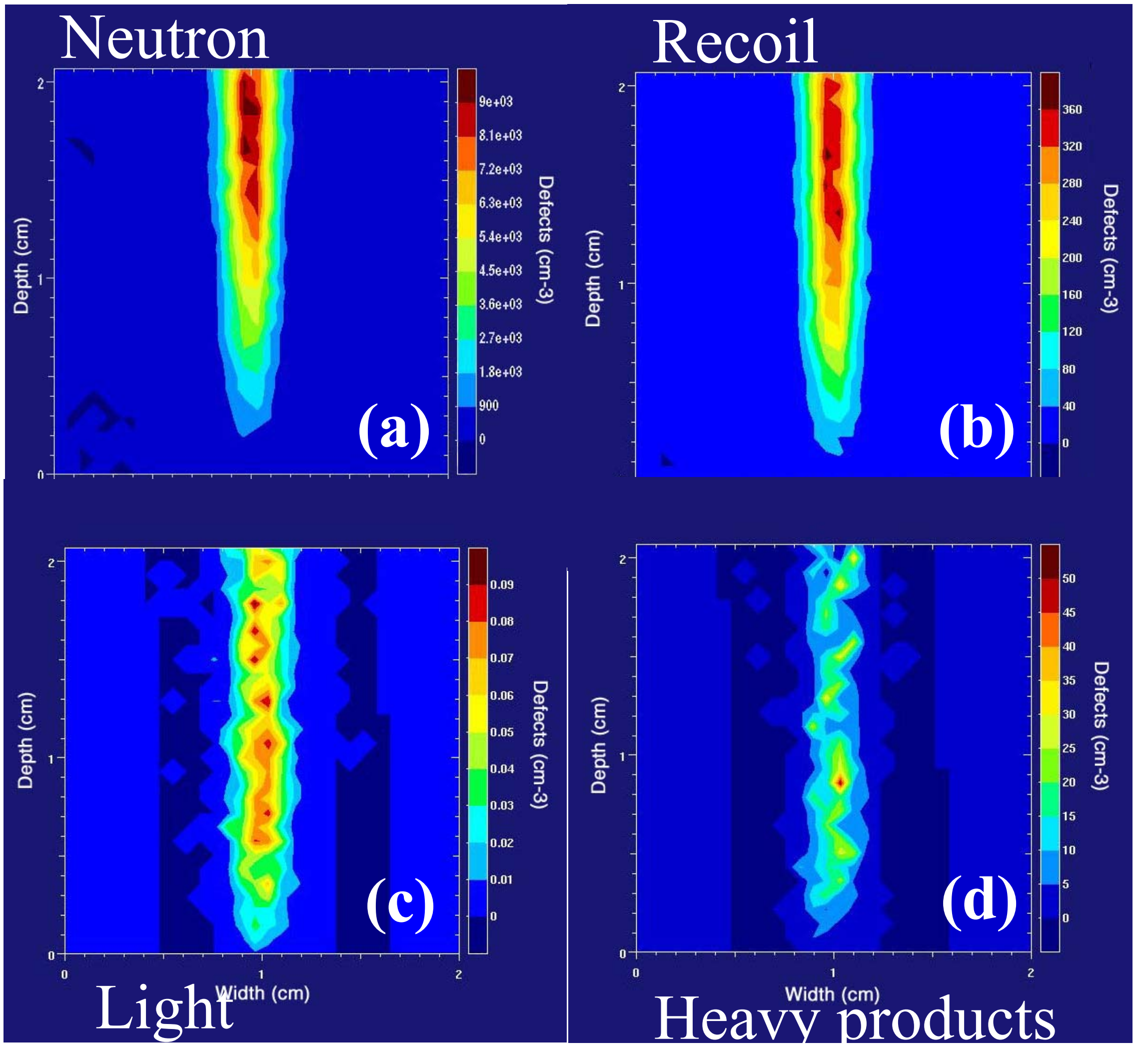

Neutron
Recoil
Light
Heavy products
(a)
(b)
(c)
(d)
Depth (cm)
Width (cm)
Defects (cm-3)
9e+03
8.1e+03
7.2e+03
6.3e+03
5.4e+03
4.5e+03
3.6e+03
2.7e+03
1.8e+03
900
0
360
320
280
240
200
160
120
80
40
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
50
45
40
35
30
25
20
15
10
5

Figure 5

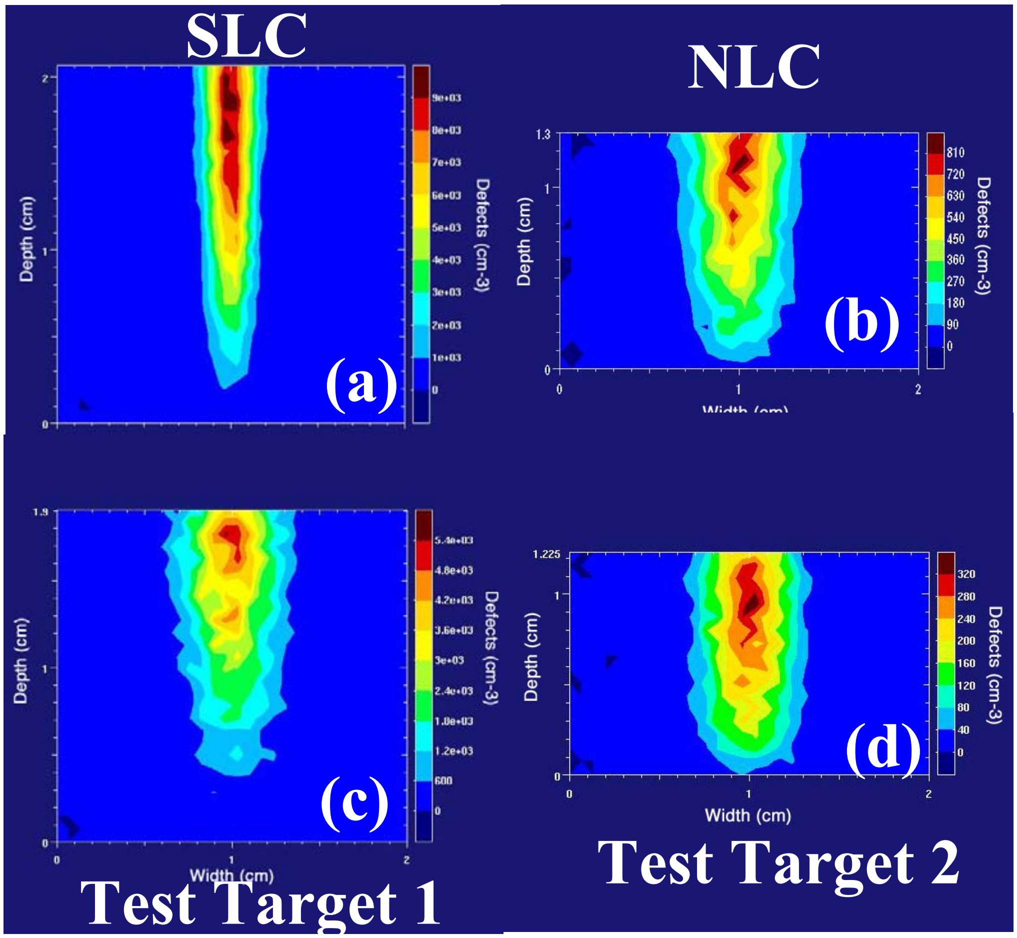
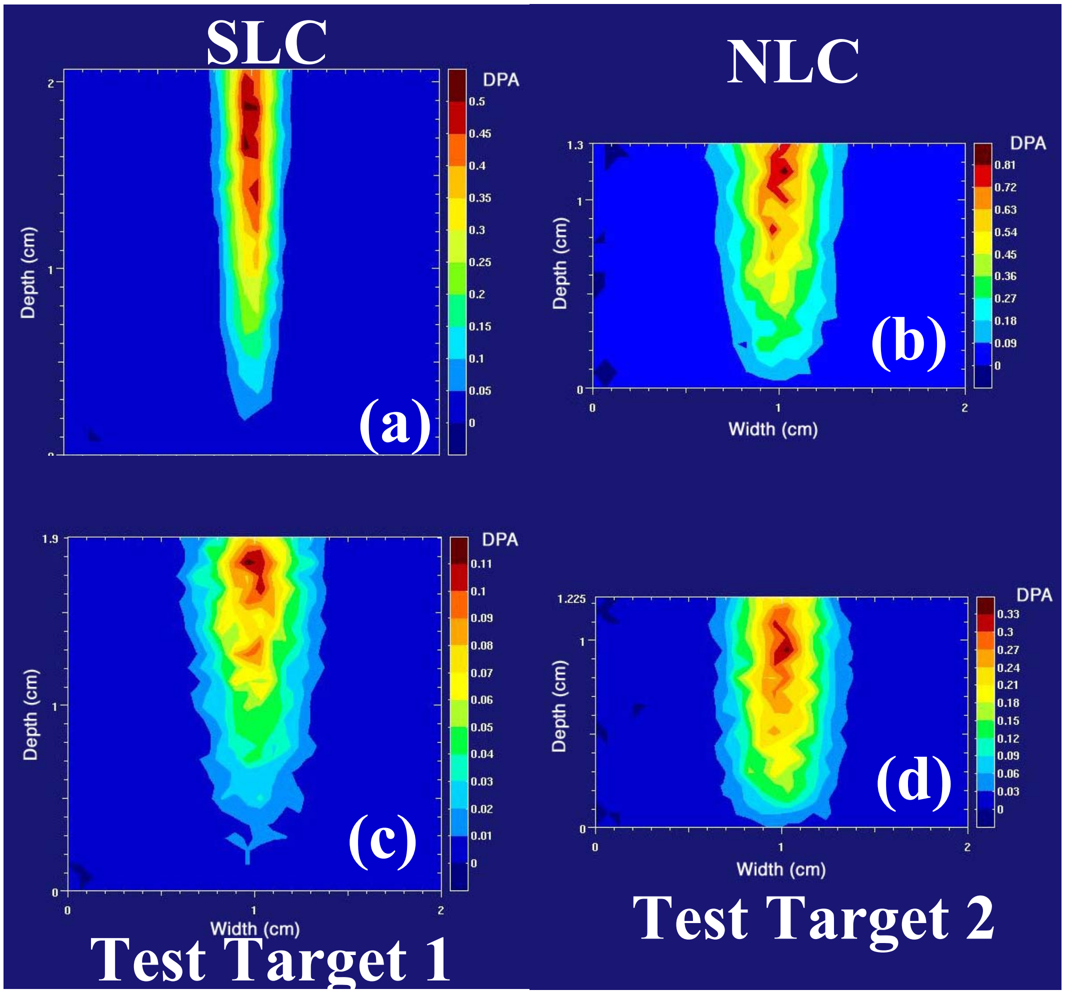

SLC
NLC
(a)
(b)
(c)
(d)
Depth (cm)
Width (cm)
Defects (cm-3)
Test Target 1
Test Target 2

Figure 6



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