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CALCULATION OF DISPLACEMENT, GAS, AND TRANSMUTATION PRODUCTION IN STAINLESS STEEL IRRADIATED WITH SPALLATION NEUTRONS

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ABSTRACT

Calculations using the high-energy transport code LAHET have been made for the production of displacements, helium gas, and transmuted atoms for stainless steel (Fe-18 wt% Cr-10 wt% Ni) irradiated with spallation neutrons at energies of 100 to 1600 MeV. The damage energy cross section increased from about 250 to 350 b keV for increasing neutron energies from 100 to 1600 MeV with a spallation spectrum average of 281 barns-keV. For a displacement threshold energy of 33 eV, the corresponding spectrum-average displacement cross section is 3400 barns. The PKA spectrum was found to be fairly independent of the incident neutron energy, with an average damage energy of 0.25-0.30 MeV. The helium production cross section increased monotonically with increasing neutron energy, with a spectrum average of 0.32 barns. The maximum transmutation yield was observed near manganese (Z = 25), corresponding to a production cross section of about 0.2 barns. Relevance to fusion materials is discussed.

DISCLAIMER

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Introduction

Spallation in the context of radiation effects on materials refers to the process whereby particles and photons are ejected from nuclei upon bombardment by high-energy protons and neutrons. Spallation neutrons, in particular, are produced when linear accelerator protons bombard the beam stop or other materials in the path of the proton beam. Measurements and calculations for the spallation neutrons produced upon 800-MeV proton bombardment at the Los Alamos Spallation Radiation Effects Facility (LASREF) have shown that the resulting neutron spectrum consists essentially of a degraded fission spectrum plus a high-energy tail that extends up to the energy of the incident protons [1-6]. The effects of LASREF irradiation on materials properties are of three types: displacement, gas (particularly helium), and transmuted atom production. Calculations of these radiation effects on copper were presented earlier for spallation neutrons by Wechsler et al. [7] and for 800-MeV protons by Coulter et al. [8] The purpose of this paper is to extend these calculations to stainless steel using newer computer codes that are now available. Of special interest is the extent to which spallation neutron sources may be useful for studying radiation effects in practical fusion reactor materials like stainless steel.

The primary computational tool used is the Los Alamos High Energy Transport Code, LAHET [9]. In the model embraced by LAHET, spallation reactions take place in two stages: (1) intranuclear cascade and (2) evaporation or fission. The principal mechanism by which energy is transferred to lattice atoms is through atom recoil attending the intranuclear cascade, evaporation and fission. The stainless steel target specimen studied in the present work was Fe-18 wt% Cr-10 wt% Ni, which is the alloy chosen earlier by Doran [10] for displacement calculations due to neutrons of energies below about 15 MeV where spallation is not expected to play a major role. The target was 50 cm in diameter and one cm thick, and each computational run consisted of 20,000 neutrons incident along the specimen axis.

Displacement Production

Since [9] was published, a new option has been added to LAHET that provides recoil energy (energy transferred to lattice atoms, including energy transferred to electrons) and damage energy (energy delivered to nuclei only and therefore fully effective in producing displacements, based on the Lindhard energy partition model [11-13]). In addition, LAHET gives the corresponding recoil and damage energy distributions or PKA spectra. Furthermore, LAHET supplies a separate tally of the PKA spectra resulting from elastic interactions. In all cases studied in the present work, the energy transferred to lattice atoms due to elastic interactions is a small fraction of the total energy. Fig. 1 shows for Fe-18 wt% Cr-10 wt% Ni the damage energy and displacement cross sections as calculated by LAHET for incident neutron energies of 100-1600 MeV and as presented by Doran [Table III in 10]. At Doran's highest incident neutron energy, 14.9 MeV, the damage energy cross section is about 290 barns-keV. At this energy, displacement production is dominated by inelastic neutron scattering and especially (n,2n) reactions. By contrast, the LAHET damage energy cross section due to spallation reactions (intranuclear cascade followed by evaporation or fission) is only about 200 barns-keV at 100 MeV, rising to about 300 barns-keV at 1600 MeV. Preliminary LAHET calculations suggest that the damage energy cross section increases again with decreasing neutron energy below 100 MeV, but further work is required to specify this behavior more definitely.

The cross sections shown in fig. 1 were folded into the spallation neutron flux spectrum appropriate to the beam stop of the LAMPF 800-MeV proton linear accelerator at the Los Alamos National Laboratory (copper beam stop, radius 10.5 cm; see, for example, fig. 3a of [6]). The spectrum-average damage energy and displacement cross sections (using a threshold displacement energy of 33 eV [10]) for the lower energy Doran section of the figure are 240 barns-keV and 2910 barns, respectively. The corresponding cross sections for the higher energy LAHET results are 281 barns-keV and 3400 barns, respectively.

As mentioned above, LAHET also provides PKA spectra. Fig. 2 shows the damage energy PKA spectra for the Fe-18 wt% Cr-10 wt% Ni alloy for incident neutron energy of 800 MeV. The average damage energy for the recoiling atoms is 0.28 MeV. The PKA damage energy spectra do not appear to be a function of the incident neutron energy in the range studied. Thus, for neutron energies of 100, 400, 800, and 1600 MeV, the average damage energy was found to be 0.27, 0.30, 0.28, and 0.25 MeV, respectively. For lower incident neutron energies, PKA spectra are given for iron in the report by Doran and Graves [14]; the average transferred energy for 13.5 MeV incident neutrons deduced from Table 14 in [14] is about 0.22 MeV. It appears, therefore, that the energies of the recoiling atoms effective in producing displacements are not greatly different for 13.5 MeV neutrons appropriate for fusion reactor applications and 100-1600 MeV neutrons present in spallation neutron flux spectra. This statement should be tested, however, with calculations that apply to the same material throughout and that are analyzed on a strictly comparable basis.

Helium Production

Helium production is, of course, an important consideration for materials used in radiation environments because of the grain boundary embrittlement that attends the formation of helium bubbles. Fig. 3 shows LAHET results for the helium production cross section as a function of incident neutron energy for the Fe-18 wt% Cr-10 wt% Ni stainless steel. The cross section appears to be roughly linear with incident neutron energy in the 100-1600 MeV range studied, extending from about 0.04 to 0.5 barns. The spallation spectrum-average cross section is calculated to be 0.32 barns.

Transmuted Atom Production

Fig. 4 gives the transmutation yield (number of transmutation product atoms of the indicated atomic number) per incident neutron and the transmutation production cross section versus atomic number for incident neutron energies of 100, 400, 800, and 1600 MeV. The greatest production occurs for Z = 24 (chromium) or 25 (manganese). For these elements the production cross section is about 0.2 barns over the entire range of incident energies.

Discussion

As indicated in [6], the neutron flux presently achieved at LAMPF is about 5×10^{17} neutrons/m^2s (E>1 keV), and this flux could be increased to 4.2×10^{18} neutrons/m^2s by decreasing the diameter of the beam stop by a factor of 2, changing the beam stop material from copper to tungsten, and removing the isotope production targets in the region of the beam stop. This would bring the neutron flux to the approximate level anticipated for ITER [15]. With the spallation spectrum-average displacement cross sections given above, the flux-enhanced displacement production rates for the lower (Doran) and upper (LAHET) energy regions in fig. 1 are 1.2×10^{-6} and 1.4×10^{-6} displacements per s per atom, respectively. One year's irradiation would give, then, 39 and 45 DPA, respectively, although a practical assessment of what is achievable in one calendar year would, of course, have to take the duty factor into account. Also, the above estimates do not include the displacements due to neutrons in the region above 14.9 MeV where Doran's calculations leave off and below 100 MeV where our LAHET calculations start.

Another question that bears on the suitability of accelerator-produced spallation neutrons for fusion materials research is the PKA spectrum. As noted above, the PKA spectra from LAHET do not appear to be sensitive to the energy of the incident neutrons in the 100-1600 MeV range. The average damage energy for these spectra for the stainless steel is in the range 0.25-0.3 MeV, which is not very different than the average energy of 0.22 MeV calculated for iron exposed to 13.5 MeV neutrons using information from the Doran and Graves report [14]. This suggests that the damage due to fusion and spallation neutrons would compare favorably, but the comparison between PKA spectra due to the two neutron spectra is a matter that needs further investigation.

As to helium production, we have seen that the calculated spallation spectrum-average helium production cross section is about 0.32 barns. In the flux-enhanced spallation neutron facility, this would correspond to a production rate of $1.3x10^{-4}$ appm He per s per atom or for a year's irradiation about 4200 appm He. The ratio of helium and displacement rates is sometimes considered to be a significant factor in determining radiation damage characteristics. Adding the displacement production rates for the Doran and LAHET sections of fig. 1 for the flux-enhanced spallation facility, we obtain a total displacement production rate of $2.65x10^{-6}$ DPA/s. The helium to displacement production ratio is, therefore, 50 appm He/DPA. Conn [16] indicated that for 316 stainless steel the ratio of helium to displacement production is 15 appm He/DPA for fusion reactors.

The production of transmuted atoms is likely to be an important factor in spallation-neutron-irradiated fusion materials. As noted above, fig. 4 indicates that the production cross section for the highest yield transmutation products is about 0.2 barns over the 100-1600 MeV neutron range. For the flux-enhanced spallation source, this corresponds to a concentration production rate of 8.4×10^{-11} per s per atom, or for a one year's irradiation a concentration of 2.7×10^{-3} or 0.27%. In stainless steel, the production of chromium at this rate should be innocuous, but there may be other transmutation induced impurity atoms that affect properties more seriously.

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Figure Captions

1. Damage energy cross section and displacement cross section (based on threshold displacement energy of 33 eV) versus incident neutron energy for Fe-18 wt% Cr-10 wt% Ni stainless steel. The Doran curve is based on Table III of [10] and the LAHET curve is present work using the Los Alamos High Energy Transport Code.

2. PKA spectrum for damage energy (differential scattering cross section with respect to damage energy versus damage energy) for Fe-18 wt% Cr-10 wt% Ni stainless steel irradiated by 800 MeV neutrons.

3. Helium production cross section versus incident neutron energy for Fe-18 wt% Cr-10 wt% Ni stainless steel.

4. Transmutation yield per incident neutron and transmutation production cross section versus atomic number Z of the transmutation product in Fe-18 wt% Cr-10 wt% Ni stainless steel irradiated by 100, 400, 800, and 1600 MeV neutrons.

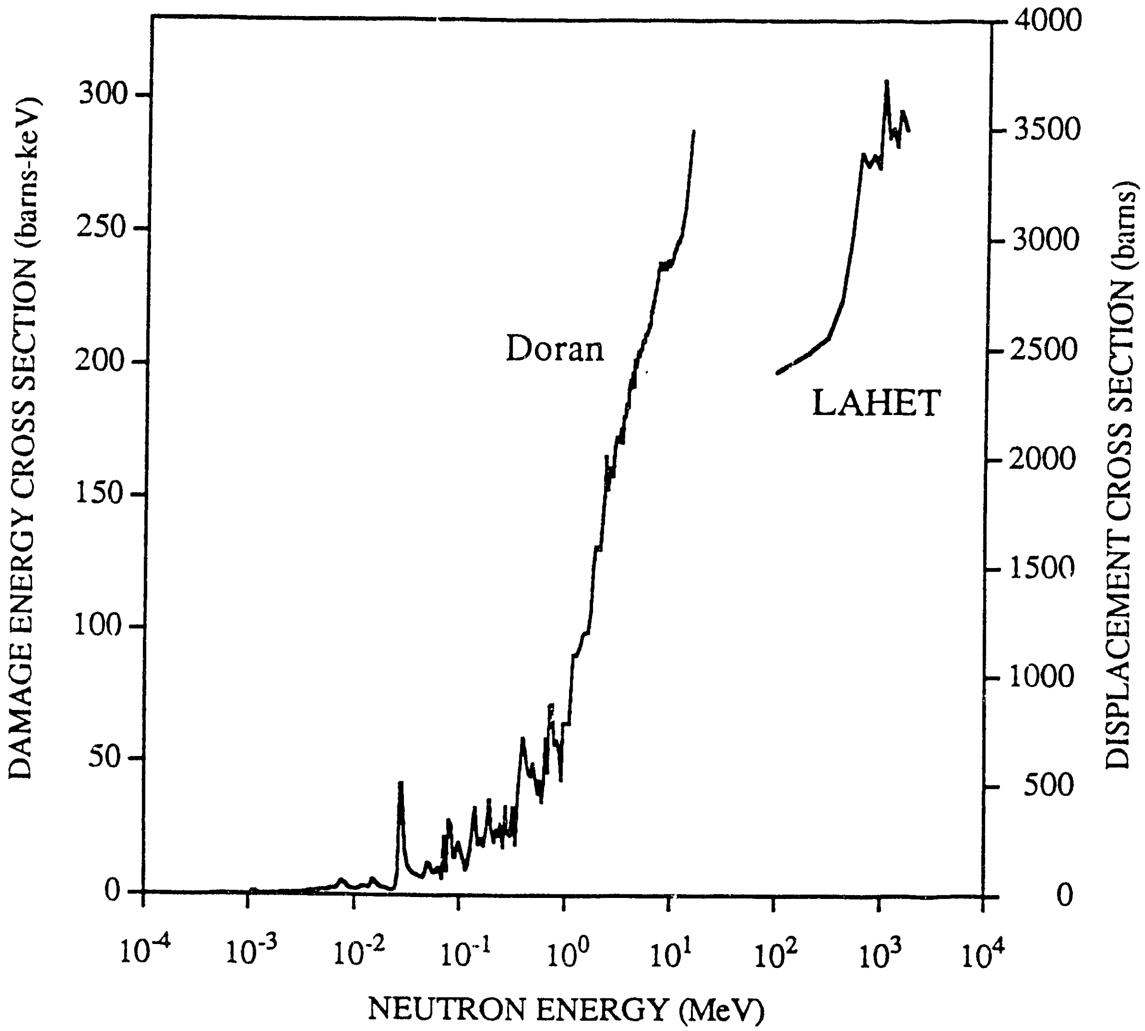
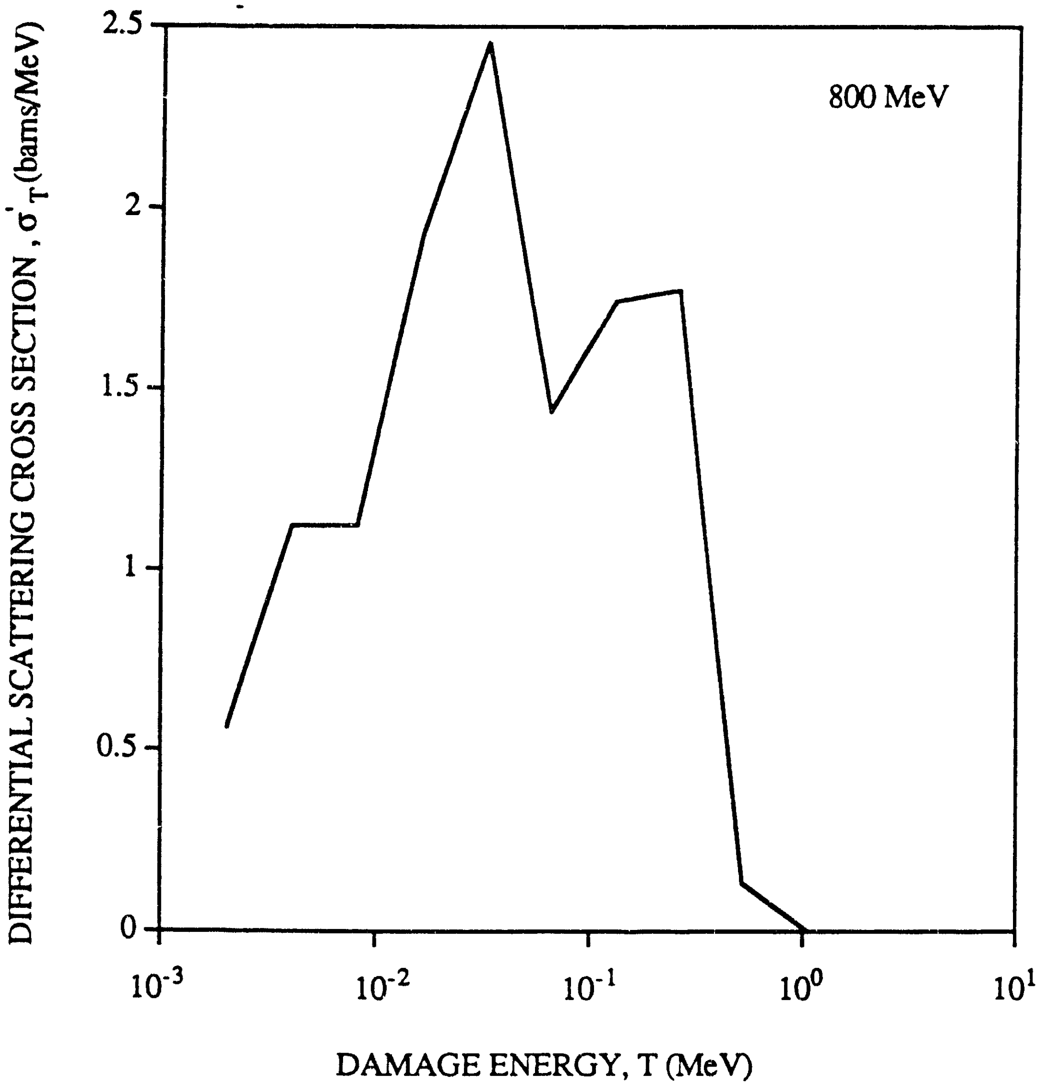
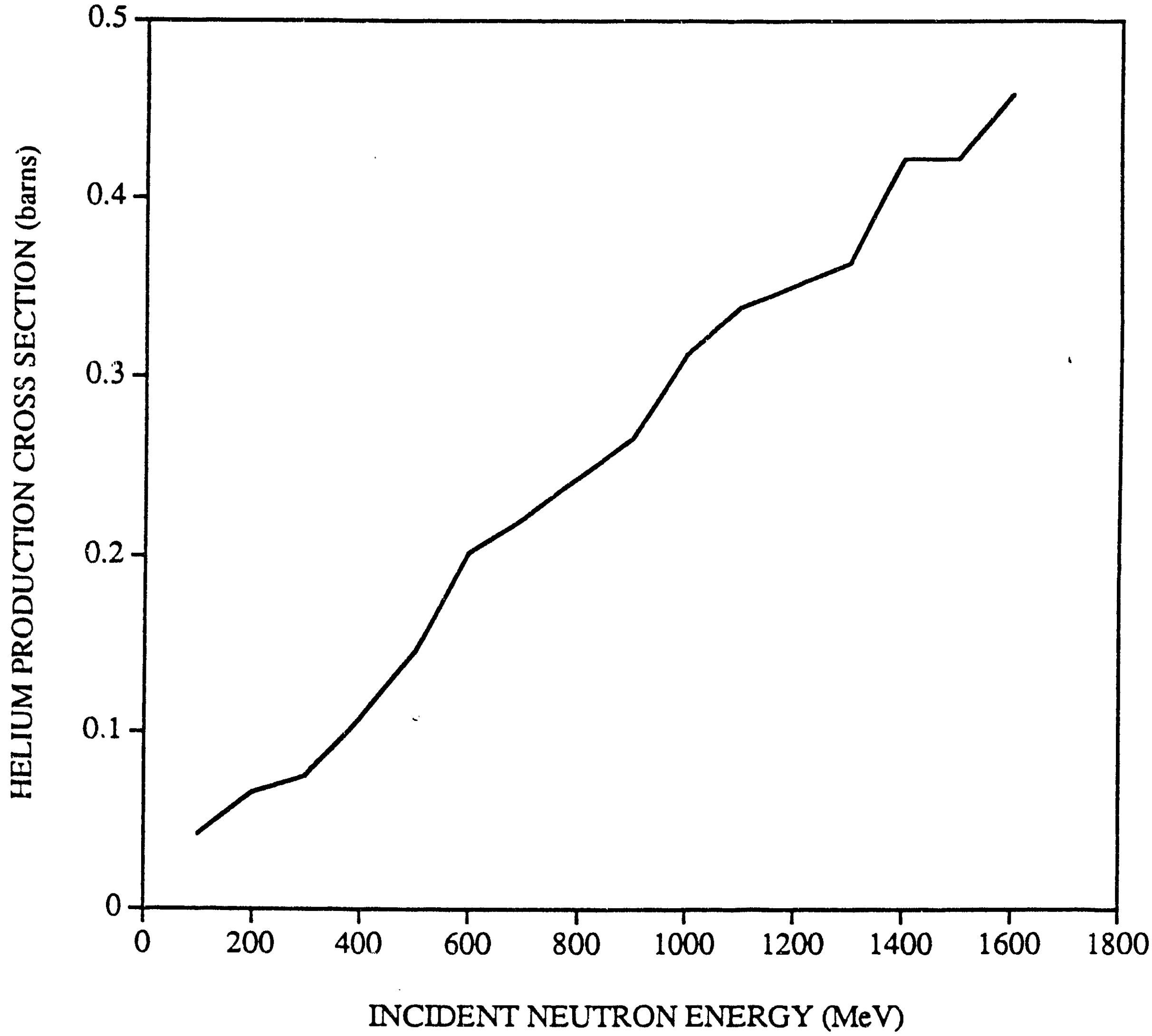

DAMAGE ENERGY CROSS SECTION (barns-keV)
300
250
200
150
100
50
0
DISPLACEMENT CROSS SECTION (barns)
4000
3500
3000
2500
2000
1500
1000
500
0
Doran
LAHET
10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2} 10^{3} 10^{4}
NEUTRON ENERGY (MeV)

FIG. 1



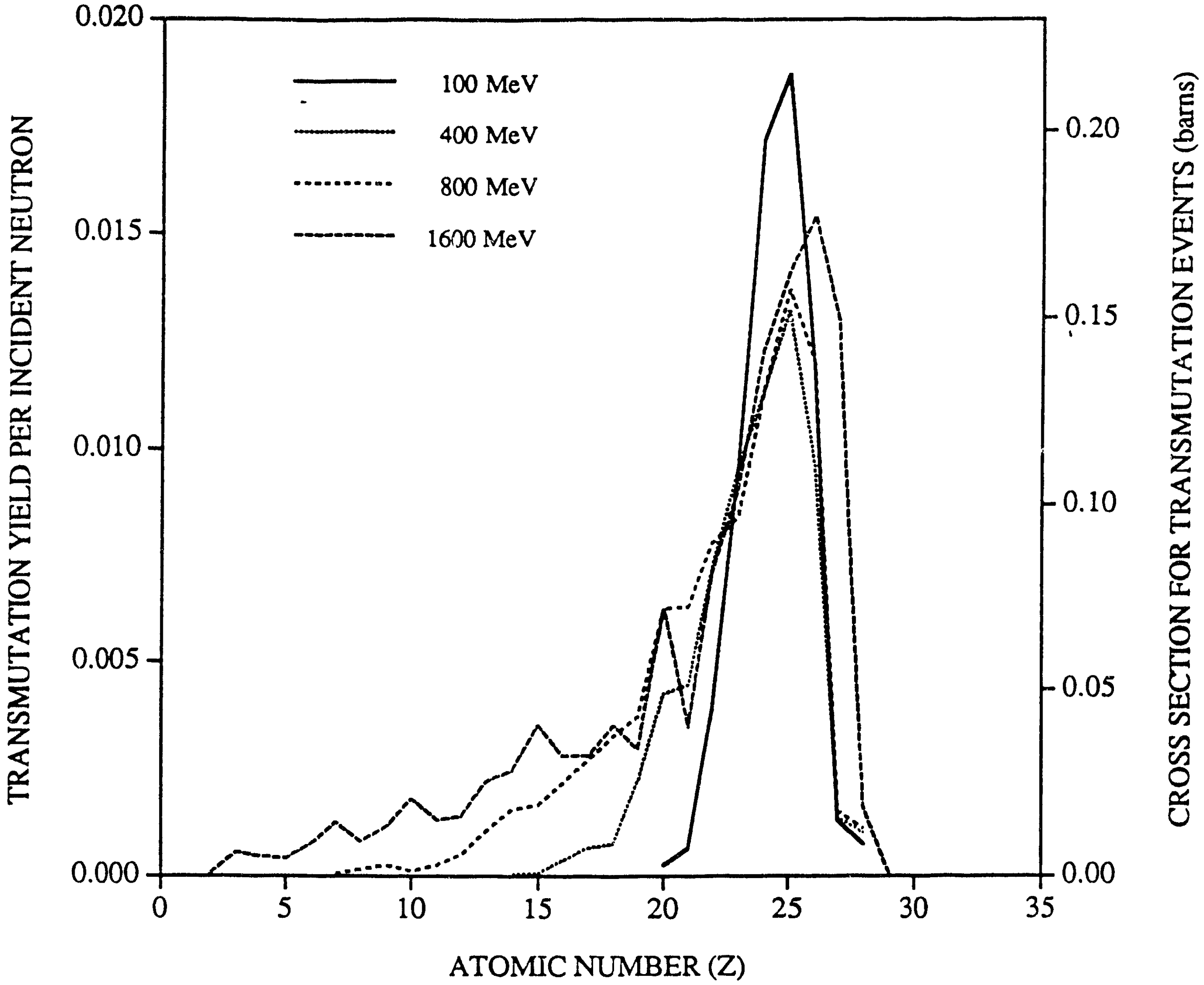
DIFFERENTIAL SCATTERING CROSS SECTION , σ'T (barns/MeV)
2.5
2
1.5
1
0.5
0
800 MeV
10-3
10-2
10-1
100
101
DAMAGE ENERGY, T (MeV)

FIG. 2



HELIUM PRODUCTION CROSS SECTION (barns)
0.5
0.4
0.3
0.2
0.1
0
0
200
400
600
800
1000
1200
1400
1600
1800
INCIDENT NEUTRON ENERGY (MeV)

FIG. 3



0.020
0.015
0.010
0.005
0.000
TRANSMUTATION YIELD PER INCIDENT NEUTRON
100 MeV
400 MeV
800 MeV
1600 MeV
0.20
0.15
0.10
0.05
0.00
CROSS SECTION FOR TRANSMUTATION EVENTS (barns)
0
5
10
15
20
25
30
35
ATOMIC NUMBER (Z)

FIG. 4

END

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