

NATIONAL INSTITUTE FOR FUSION SCIENCE**Sputtering Yield Formula for B₄C Irradiated with Monoenergetic Ions at Normal Incidence**

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Erratum: eq.(6) on p.4 is to be replaced by

$$\begin{aligned} \alpha^* &= 0.249(M_k/M_1)^{0.56} + 0.0035(M_k/M_1)^{1.5} & M_1 \leq M_k \\ &= 0.088(M_k/M_1)^{-0.15} + 0.165(M_k/M_1) & M_1 \geq M_k \end{aligned} \quad (6)$$

Sputtering Yield Formula for B₄C Irradiated with Monoenergetic Ions at Normal Incidence

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Abstract

To fill a lack in sputtering yield data for a B₄C material which may be a promising plasma-facing material in fusion devices, yields of H⁺, D⁺, T⁺, He⁺, B⁺, C⁺, Ne⁺, Ar⁺ and Kr⁺ ions were calculated for this multi-component material for normal incidence with a computer simulation code ACAT. A fitting formula of sputtering yield for a B₄C was proposed based on an empirical formula for monoatomic target materials at normal incidence. By fitting the formula to the calculated data, best-fit values of the parameters included in it were derived for the material. Good agreement was found between the formula and the data. Thus, the formula proposed for the multi-component material provides a way to estimate the erosion of a B₄C material irradiated with above ions at normal incidence. Preferential sputtering for this material was also mentioned briefly

KEYWORDS: physical sputtering, boron carbide, fitting formula, normal incidence, preferential sputtering

1. Introduction

In fusion devices the areas of the materials facing a plasma have to receive large fluxes of energy and particles. For a magnetically confined plasma, these fluxes are concentrated on divertor plates or limiters, so that these materials may be seriously damaged and eroded. Impurities, which are the constituents of the materials, are then generated through erosion. Impurity reduction is an important problem for fusion plasmas, since impurities introduced then into a core plasma cause core plasma cooling by radiation and dilution of the fuel. To prevent accumulation of impurities in a core plasma, erosion of plasma-facing materials in a fusion device should be very low.

Boronization, a recently developed wall conditioning, is a thin boron coating onto plasma-facing surfaces using a boron-containing gas mixture. Boronization executed in major tokamaks has proved to be effective to reduce metallic impurities and oxygen as well.¹⁻⁶⁾ The thickness of the boron layers used was usually limited to an order of several 100nm. However, such thin layers are not sufficient to keep lower the impurity level and recycling hydrogen for many high-power discharges. Hence, a few hundred micrometers thick B_4C layers have been prepared and investigated on their hydrogen retention characteristics.⁷⁾ It was shown that B_4C has a lower release temperature of implanted deuterium than graphite which is a commonly used plasma-facing material in fusion devices. In addition, B_4C was installed in the tokamaks as divertor tiles or coatings.^{8,9)} By the combined effects of boronization with decaborane and the boron burst from the B_4C tiles, oxygen impurity was reduced to the noise detection level.⁸⁾ The B_4C coatings also showed excellent durability under a real tokamak divertor plasma.⁹⁾ Thus, B_4C is thought to be one of the potential candidates for plasma-facing materials in fusion devices.

Sputtering is one of the main processes of erosion of a material exposed to ion bombardment. Sputtering yield depends strongly on the incident energy of a projectile. Hence, it is important to know energy dependence of ion-induced sputtering yield of plasma ions for B_4C . The experimental data available now are not enough for the purpose. To fill a lack in the yield data for this material, sputtering yield was calculated for nine kinds of ions at normal incidence. The ions are H^+ , D^+ , T^+ , He^+ , B^+ , C^+ , Ne^+ , Ar^+ and Kr^+ . The calculations were done for the multi-component target with a Monte Carlo simulation code ACAT¹⁰⁾ in a wide range of incident energy. The calculated data of sputtering yield will be compared with the experimental data. Then, based on a Yamamura and Tawara formula¹¹⁾ that represents sputtering yield for monoatomic target materials at normal incidence, a fitting formula of sputtering yield for a B_4C material will be proposed. By fitting the formula to above calculated data, four unknown parameters included in the formula will be determined. In particular, sputtering threshold energy, which is one of these parameters, will be

presented in a functional form.

Preferential sputtering for this material will also be referred to briefly.

2. Fitting Formula of Sputtering Yield for Multi-Component Materials

Based on the Yamamura and Tawara formula for monoatomic target materials, an empirical fitting formula for multi-component materials $Y(E)$ is proposed:

$$Y(E) = 0.042 \frac{Q \langle \alpha^* S_n(E) \rangle}{\langle U \rangle} \frac{1}{1 + \Gamma \langle k_e \varepsilon^{0.3} \rangle} \left[1 - \sqrt{\frac{E_{th}}{E}} \right]^s, \quad (1)$$

where the factor Γ has the following form:

$$\Gamma = \frac{W}{1 + (M_1/\bar{M})^3}, \quad (2)$$

where M_1 is the mass of a projectile in u: E is the incident energy of a projectile: E_{th} is the sputtering threshold energy: the numerical factor is expressed in units of \AA^{-2} : Q , W , E_{th} and s are the fitting parameters of a target material: among those, Q and W depend on a target material, while E_{th} is a function of a mass ratio of a projectile and a mean mass of atoms in a target material: the latter mass is defined as

$$\langle M_2 \rangle = \sum_k c_k M_k, \quad (3)$$

where c_k and M_k are the constituent ratio and the mass of a k -atom of a multi-component material: the power s in eq.(1) is slightly dependent on both a projectile and a target material: the physical quantities other than Q , W , E_{th} and s in eqs.(1) and (2) are derived uniquely from the ones for a monoatomic material: $\langle U \rangle$ is the effective surface binding energy of a multi-component material and it is defined as

$$\langle U \rangle = \sum_k c_k U_k, \quad (4)$$

where U_k means the surface binding energy of a pure k -material: the term $\langle \alpha^* S_n \rangle$ is calculated as

$$\langle \alpha^* S_n(E) \rangle = \sum_k c_k \alpha^*(M_k/M_1) S_{nk}(E), \quad (5)$$

where the best-fit values of α^* are given for monoatomic materials as a function of a mass ratio M_k/M_1 in the form of^{f11)}

$$\begin{aligned}\alpha^* &= 0.249(M_k/M_1)^{0.56} + 0.0035(M_k/M_1)^{1.5} & M_1 \geq M_k \\ &= 0.088(M_k/M_1)^{-0.15} + 0.165(M_k/M_1) & M_1 \leq M_k\end{aligned}\quad (6)$$

$S_{nk}(E)$ is the nuclear stopping cross-section of a k -atom and it is expressed as

$$S_{nk}(E) = 84.78 \frac{Z_1 Z_k}{(Z_1^{2/3} + Z_k^{2/3})^{1/2}} \frac{M_1}{M_1 + M_k} s_n^{\text{TF}}(\varepsilon_k) \quad , \quad (7)$$

in units of eV Å²/atom: Z_k is the atomic number of a k -atom: $s_n^{\text{TF}}(\varepsilon_k)$ is the reduced nuclear stopping cross-section and it is approximated¹²⁾ by

$$s_n^{\text{TF}}(\varepsilon_k) = \frac{3.441\sqrt{\varepsilon_k} \ln(\varepsilon_k + 2.718)}{1 + 6.355\sqrt{\varepsilon_k + \varepsilon_k}(6.882\sqrt{\varepsilon_k} - 1.708)} \quad , \quad (8)$$

where ε_k is a reduced energy and it is given by

$$\varepsilon_k = \frac{0.03255}{Z_1 Z_k (Z_1^{2/3} + Z_k^{2/3})^{1/2}} \frac{M_k}{M_1 + M_k} E \text{ (eV)} \quad . \quad (9)$$

The term $\langle k_e \varepsilon^{0.3} \rangle$ is given as

$$\langle k_e \varepsilon^{0.3} \rangle = \sum_k c_k k_{ek} \varepsilon_k^{0.3} \quad , \quad (10)$$

where k_{ek} is the Lindhard electronic stopping coefficient¹³⁾ of a k -atom and it is defined as

$$k_{ek} = 0.079 \frac{(M_1 + M_k)^{3/2}}{M_1^{3/2} M_k^{1/2}} \frac{Z_1^{2/3} Z_k^{1/2}}{(Z_1^{2/3} + Z_k^{2/3})^{3/4}} \quad . \quad (11)$$

3. Calculated Yield Data and Fitting Procedure

Sputtering yield of a B₄C material was calculated for monoenergetic ions with normal incidence in the energy range of a few tens to 10⁴ eV or higher. The calculations were done for the multi-component target with a Monte Carlo simulation code ACAT¹⁰⁾ that simulates atomic collisions in an amorphous target material based on a binary collision approximation. The density of a B₄C material considered is 2.52[g/cm³]. The effective surface binding energy for an i -atom in a multi-

component material U_i is given by^{14,15)}

$$U_i = \sum_k c_k U_{ik} \quad , \quad (12)$$

where

$$U_{ik} = \frac{1}{2}(U_{ii} + U_{kk}) \quad , \quad (13)$$

where U_{ii} is the nearest neighbor i - i bond strength and similarly for U_{kk} and U_{ik} ; U_{ii} and U_{kk} are approximated by the heats of sublimation of pure elemental i - and j -materials. For self-sputtering for B^+ and C^+ ions, reflection of the incident ions is not included in the yield values. The calculated data marked with stars are shown in Figs.1-9. The data marked with "A" in these figures are those obtained by experiments¹⁶⁻¹⁸⁾ and compiled by Eckstein et al.¹⁹⁾ Good agreement is seen between the calculated and the experimental data for H^+ , D^+ and C^+ ions if the data scattering is taken into account at the same energies for the experimental data. Slight differences between the ACAT data and the experiments, however, exist for He^+ and Ne^+ ions.

From eq.(2), Γ are expected to become much smaller than unity for large M_1 , considering that the values of W are 4.39 and 1.70 for B and C.¹¹⁾ From eqs (9)-(11), the term $\langle k_e \mathcal{E}^{0.3} \rangle$ can be shown easily to be also much smaller than unity for large M_1 in the energy range concerned. Because of these facts, the term $\Gamma \langle k_e \mathcal{E}^{0.3} \rangle$ in eq.(1) can be neglected for large M_1 . Thus, the best-fit values of Q , E_{th} and s are obtained first by fitting the formula to the yield data for a large M_1 . Γ approaches W in eq.(2) for small M_1 , i.e., M_1 of hydrogen or deuterium. The term $\Gamma \langle k_e \mathcal{E}^{0.3} \rangle$ affects the formula in the high energy for small M_1 . Secondly, with the use of these facts and the value of Q calculated above, the best-fit values of W , E_{th} and s are calculated by fitting the formula to the data for hydrogen or deuterium. Finally, with the values of Q and W derived above, the best-fit values of E_{th} and s are derived by fitting the formula to the data for intermediately large M_1 .

4. Results

The calculated data of sputtering yield distribute systematically over a wide range of incident

energy for all the ions considered, while the experimental data are scattered for H⁺ and D⁺ ions and are lacking for T⁺ and B⁺ ions. Hence, fitting of the yield formula was done with the calculated data. The result is shown with the thick solid lines in Figs.1-9. The power s in eq.(1) for B₄C has a best-fit functional form of

$$s = \frac{10M_1}{1+4M_1} \quad (14)$$

The best-fit values of Q and W derived by these fits are listed in Table 1, together with the other physical quantities included in the empirical formula. Through these fittings good agreement was achieved between the yield formula and the calculated data. The symbols in Fig.10 represent the best-fit values of E_{th} divided by $\langle U \rangle$. Using these data, a best-fit functional form of E_{th} was adopted:

$$\begin{aligned} \frac{E_{th}}{\langle U \rangle} &= \frac{12.12 - 5.35(\langle M_2 \rangle / M_1) + 2.2(\langle M_2 \rangle / M_1)^2}{\gamma} \quad M_1 \geq \langle M_2 \rangle \\ &= \frac{1 + 3.7(M_1 / \langle M_2 \rangle) + 4.29(M_1 / \langle M_2 \rangle)^2}{\gamma} \quad M_1 \leq \langle M_2 \rangle \end{aligned} \quad (15)$$

where $\langle M_2 \rangle$ is the mean mass of atoms in a B₄C material and it is expressed as

$$\langle M_2 \rangle = \sum_k c_k M_k \quad (16)$$

γ corresponds to the energy transfer factor for an elastic collision and it is defined as

$$\gamma = \frac{4M_1 \langle M_2 \rangle}{(M_1 + \langle M_2 \rangle)^2} \quad (17)$$

The curve shown in Fig.10 is drawn using eq.(15). From this figure, good agreement is clear between eq.(15) and above-mentioned data. The thin solid lines in Figs.1-9 mean yield curves with threshold energies calculated with eq.(15). Good agreement is seen again between the ACAT data and the empirical formula. This result indicates that sputtering yield with a B₄C material may be estimated for unlisted ions with the present empirical formula.

Preferential sputtering occurring for a B₄C material is illustrated with the case of H⁺ ion

incidence as shown in Fig.11. The circles indicate a ratio of a partial sputtering yield of boron and the total sputtering yield which was shown in Fig.1, while the squares show that of a partial sputtering yield of carbon and the total sputtering yield. This figure indicates that carbon atoms are not sputtered for incident energies lower than the sputtering threshold energy of carbon atoms. Such strong preferential sputtering will drastically modify the surface composition of a B_4C material when that material is exposed to low-temperature plasma ions for a long time.

5. Conclusion

To fill a lack in the sputtering yield data for B_4C , sputtering yields were calculated for this multi-component material with a computer-simulation code ACAT for normal incidence of H^+ , D^+ , T^+ , He^+ , B^+ , C^+ , Ne^+ , Ar^+ and Kr^+ ions. Fairly good agreement was found between the calculated and the experimental data. A fitting formula of sputtering yield for a multi-component material of a B_4C was made based on an empirical formula for monoatomic target materials at normal incidence. By fitting it to the calculated data, best-fit values of the four parameters included in the formula were derived. From comparison with the data, the formula agreed well with all the data. Thus, it provides a way to estimate the erosion of a B_4C material irradiated with above ions at normal incidence. There is no ambiguity in the formula for a projectile, because the parameters included in the formula are functions of the physical quantities of a B_4C and its constituent materials and of a mass ratio of a projectile and a mean mass of atoms in the target material. This indicates that sputtering yield of the material may be estimated for unlisted ions with the present formula. Fitting of the formula for the other multi-component materials is in progress.

It was also pointed out that strong preferential sputtering takes place for this material at incident energies lower than about 10^2 eV. A detailed study of this phenomenon for the material, in which changes of the surface composition due to ion doses are taken into account, is also in progress.

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Figure Captions

Fig.1: Energy dependence of sputtering yield of B_4C .with H^+ . The thick and thin solid lines mean yield curves with the best-fit threshold energy and that calculated by eq.(15), respectively.

$$\langle M_2 \rangle = 11.05, \langle M_2 \rangle / \langle M_1 \rangle = 10.96, Q = 1.70, \langle U \rangle = 6.09\text{eV}, W = 1.75, s = 2.00.$$

Fig.2: Energy dependence of sputtering yield of B_4C .with D^+ . The thick and thin solid lines mean yield curves with the best-fit threshold energy and that calculated by eq.(15), respectively.

$$\langle M_2 \rangle = 11.05, \langle M_2 \rangle / \langle M_1 \rangle = 5.49, Q = 1.70, \langle U \rangle = 6.09\text{eV}, W = 1.75, s = 2.22.$$

Fig.3: Energy dependence of sputtering yield of B_4C .with T^+ . The thick and thin solid lines mean yield curves with the best-fit threshold energy and that calculated by eq.(15), respectively.

$$\langle M_2 \rangle = 11.05, \langle M_2 \rangle / \langle M_1 \rangle = 3.66, Q = 1.70, \langle U \rangle = 6.09\text{eV}, W = 1.75, s = 2.31.$$

Fig.4: Energy dependence of sputtering yield of B_4C .with He^+ . The thick and thin solid lines mean yield curves with the best-fit threshold energy and that calculated by eq.(15), respectively.

$$\langle M_2 \rangle = 11.05, \langle M_2 \rangle / \langle M_1 \rangle = 2.76, Q = 1.70, \langle U \rangle = 6.09\text{eV}, W = 1.75, s = 2.35.$$

Fig.5: Energy dependence of sputtering yield of B_4C .with B^+ . The thick and thin solid lines mean yield curves with the best-fit threshold energy and that calculated by eq.(15), respectively.

$$\langle M_2 \rangle = 11.05, \langle M_2 \rangle / \langle M_1 \rangle = 1.02, Q = 1.70, \langle U \rangle = 6.09\text{eV}, W = 1.75, s = 2.44.$$

Fig.6: Energy dependence of sputtering yield of B_4C .with C^+ . The thick and thin solid lines mean yield curves with the best-fit threshold energy and that calculated by eq.(15), respectively.

$$\langle M_2 \rangle = 11.05, \langle M_2 \rangle / \langle M_1 \rangle = 0.92, Q = 1.70, \langle U \rangle = 6.09\text{eV}, W = 1.75, s = 2.45.$$

Fig.7: Energy dependence of sputtering yield of B_4C .with Ne^+ . The thick and thin solid lines mean yield curves with the best-fit threshold energy and that calculated by eq.(15), respectively.

$$\langle M_2 \rangle = 11.05, \langle M_2 \rangle / \langle M_1 \rangle = 0.55, Q = 1.70, \langle U \rangle = 6.09\text{eV}, W = 1.75, s = 2.47.$$

Fig.8: Energy dependence of sputtering yield of B_4C .with Ar^+ . The thick and thin solid lines mean yield curves with the best-fit threshold energy and that calculated by eq.(15), respectively.

$$\langle M_2 \rangle = 11.05, \langle M_2 \rangle / \langle M_1 \rangle = 0.28, Q = 1.70, \langle U \rangle = 6.09 \text{eV}, W = 1.75, s = 2.48$$

Fig.9: Energy dependence of sputtering yield of B_4C with Kr^+ . The thick and thin solid lines mean yield curves with the best-fit threshold energy and that calculated by eq.(15), respectively.

$$\langle M_2 \rangle = 11.05, \langle M_2 \rangle / \langle M_1 \rangle = 0.13, Q = 1.70, \langle U \rangle = 6.09 \text{eV}, W = 1.75, s = 2.49.$$

Fig.10: Relative sputtering threshold energy of B_4C as a function of a mass ratio $\langle M_2 \rangle / \langle M_1 \rangle$. The symbols correspond with the best-fit values of E_{th} adopted for the yield fittings.

Fig.11: Energy dependence of ratios of partial sputtering yields of B and C and total sputtering yield of B_4C . The circles correspond with the former ratio and the squares with the latter one.

Table caption

Table 1: Physical parameters included in the empirical formula.

Table 1

Q	1.70
W	1.75
$\langle U \rangle$	6.09eV
$\langle M_2 \rangle$	11.05

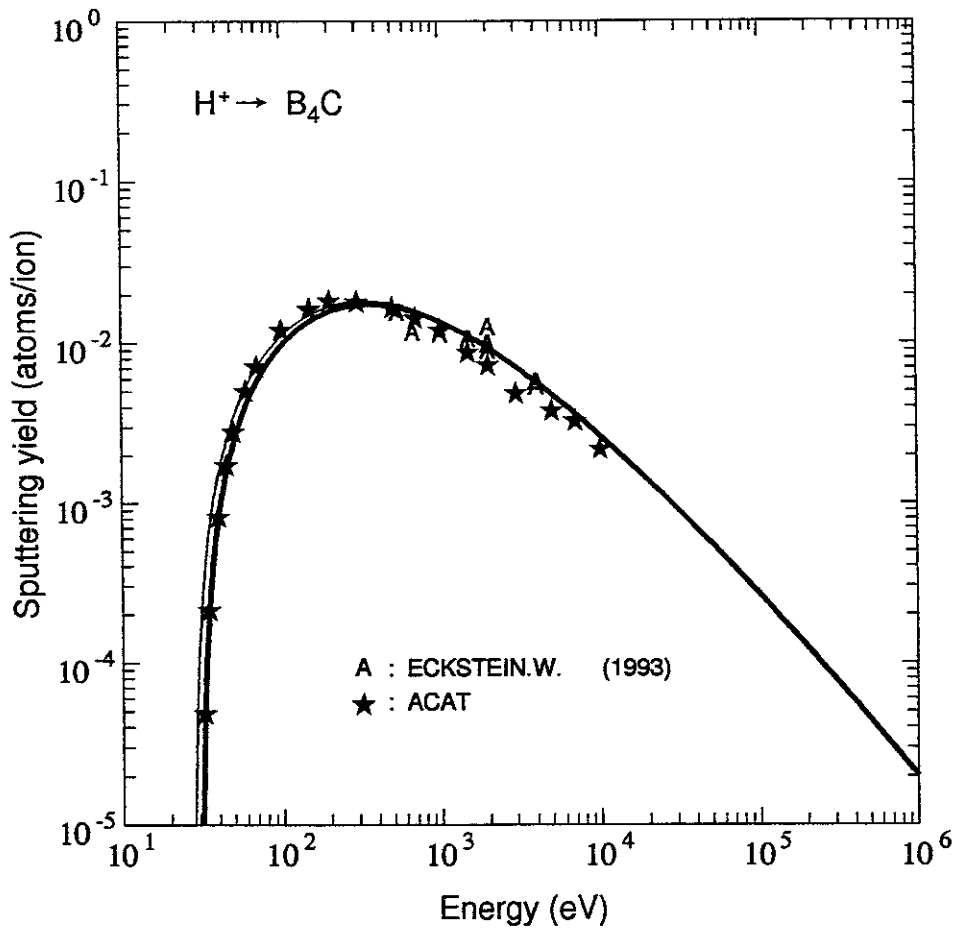


Fig. 1

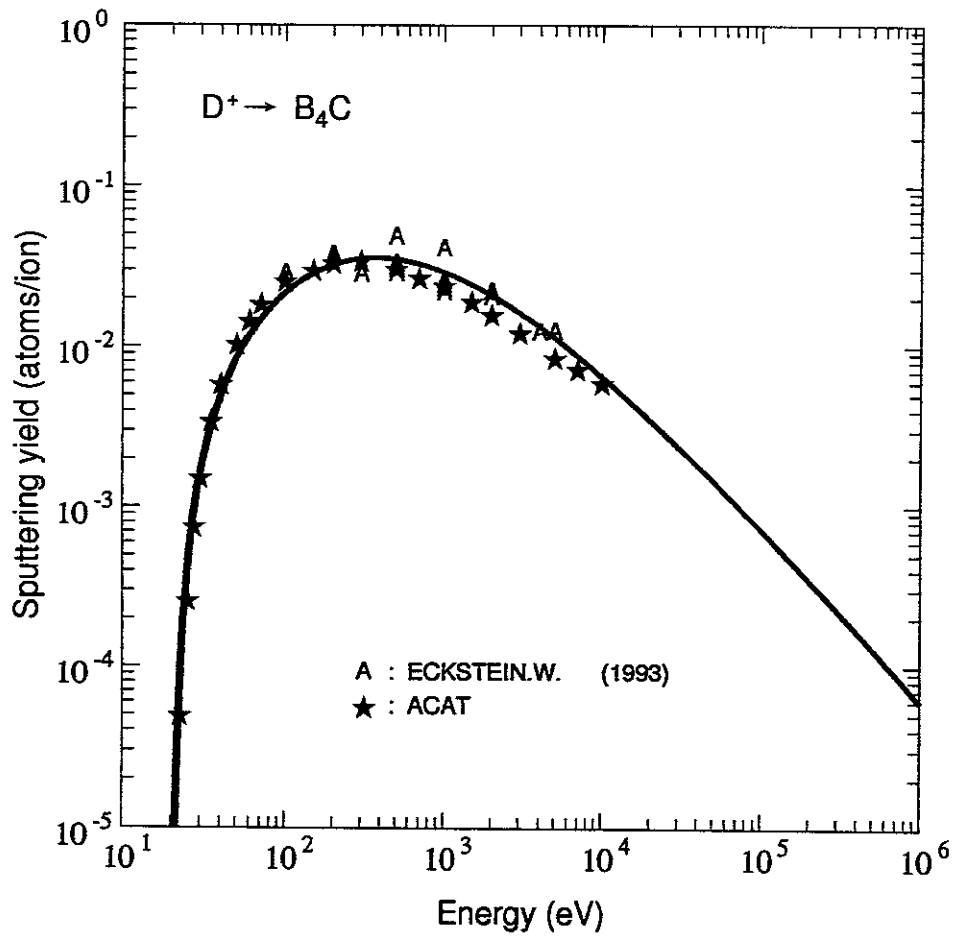


Fig. 2

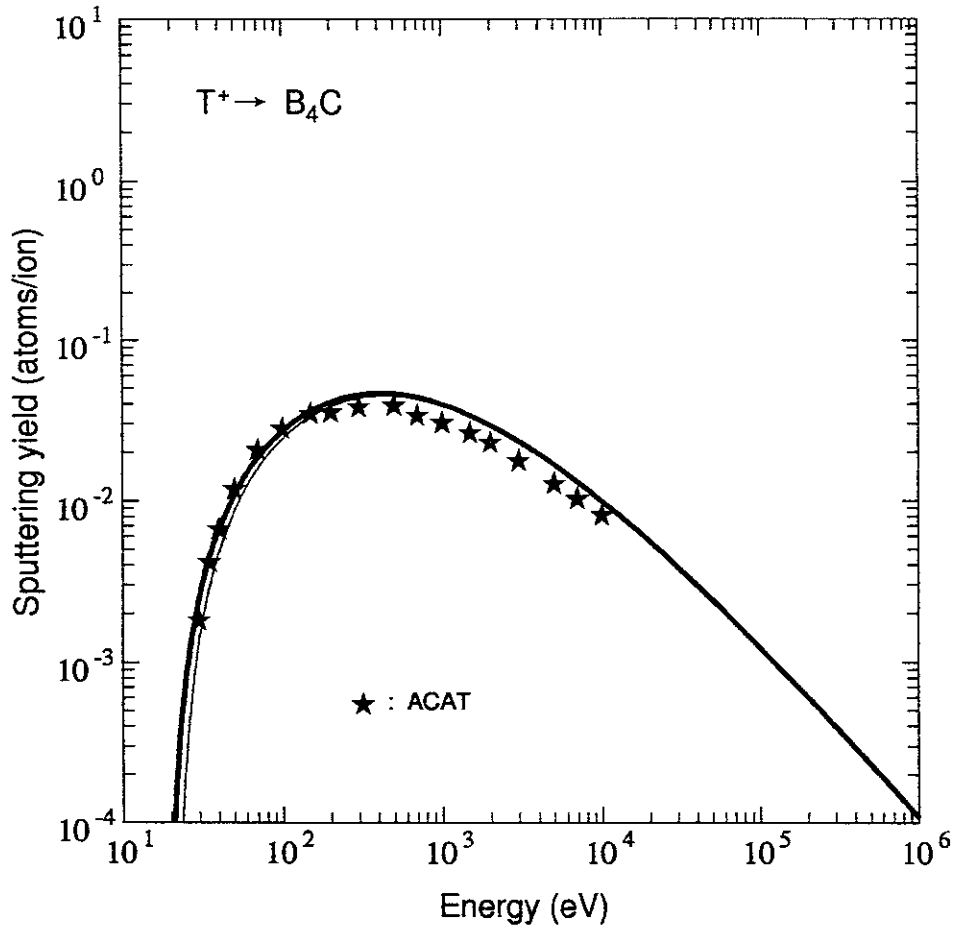


Fig. 3

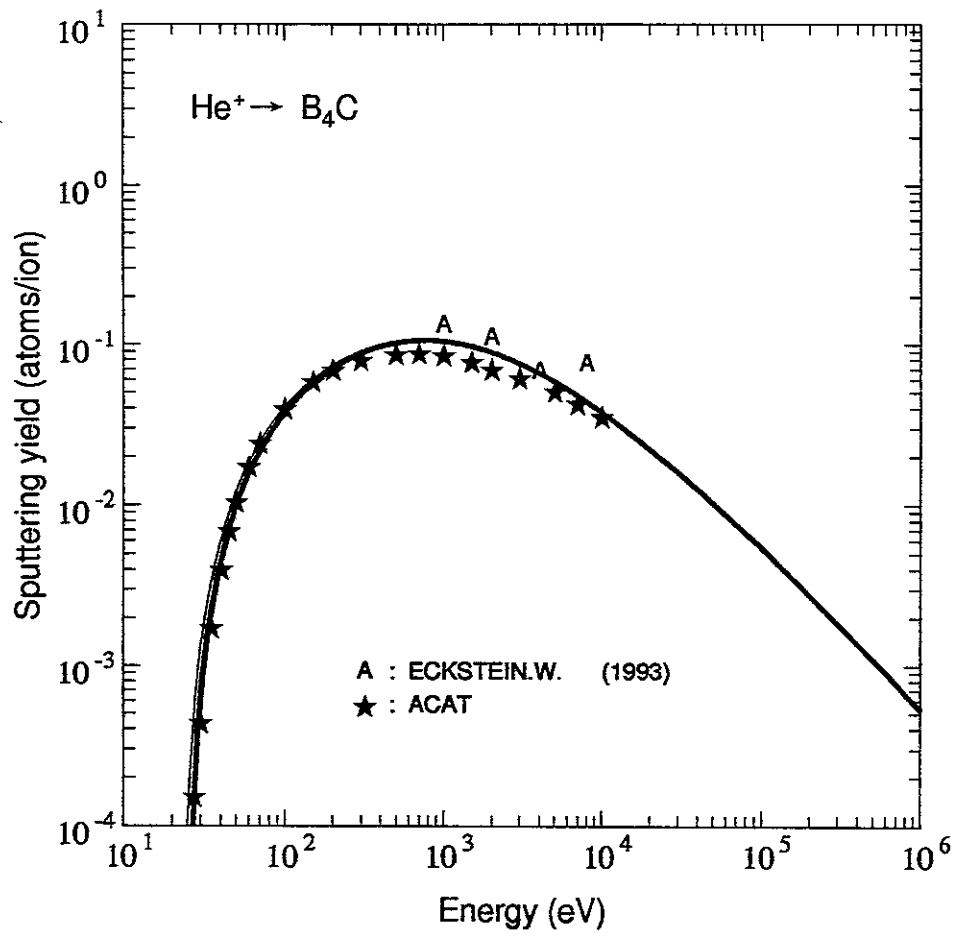


Fig. 4

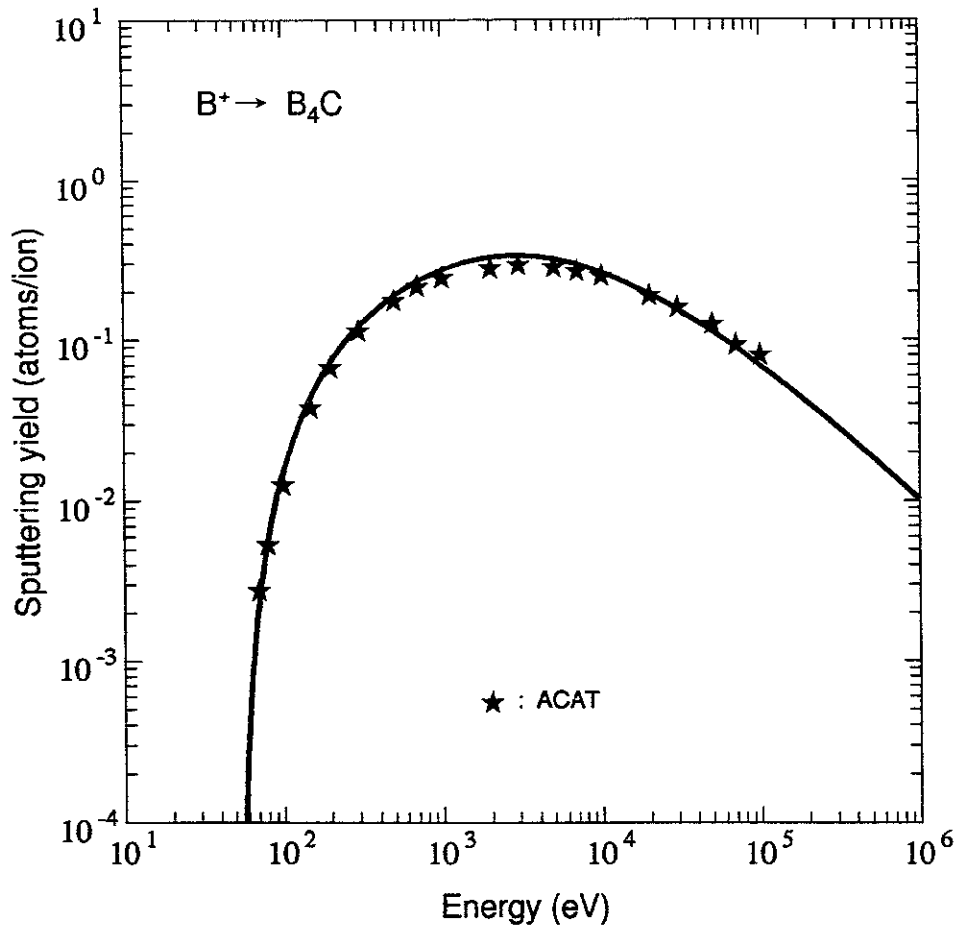


Fig.5

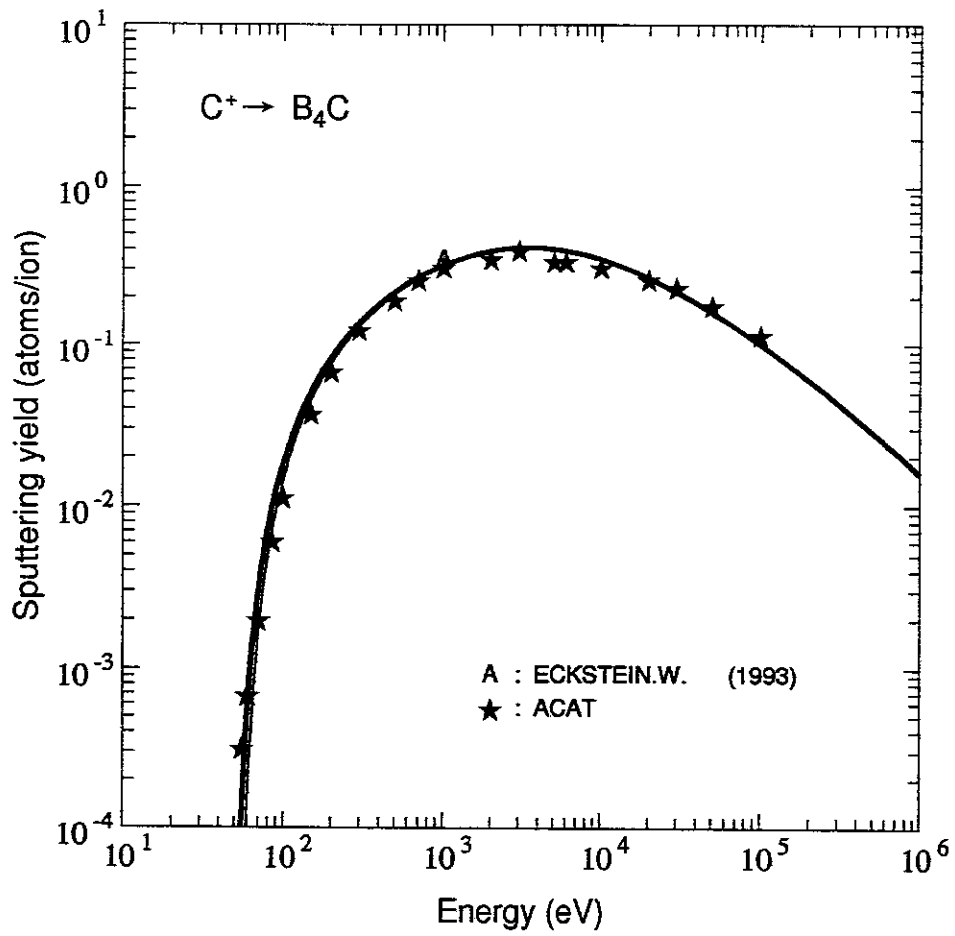


Fig.6

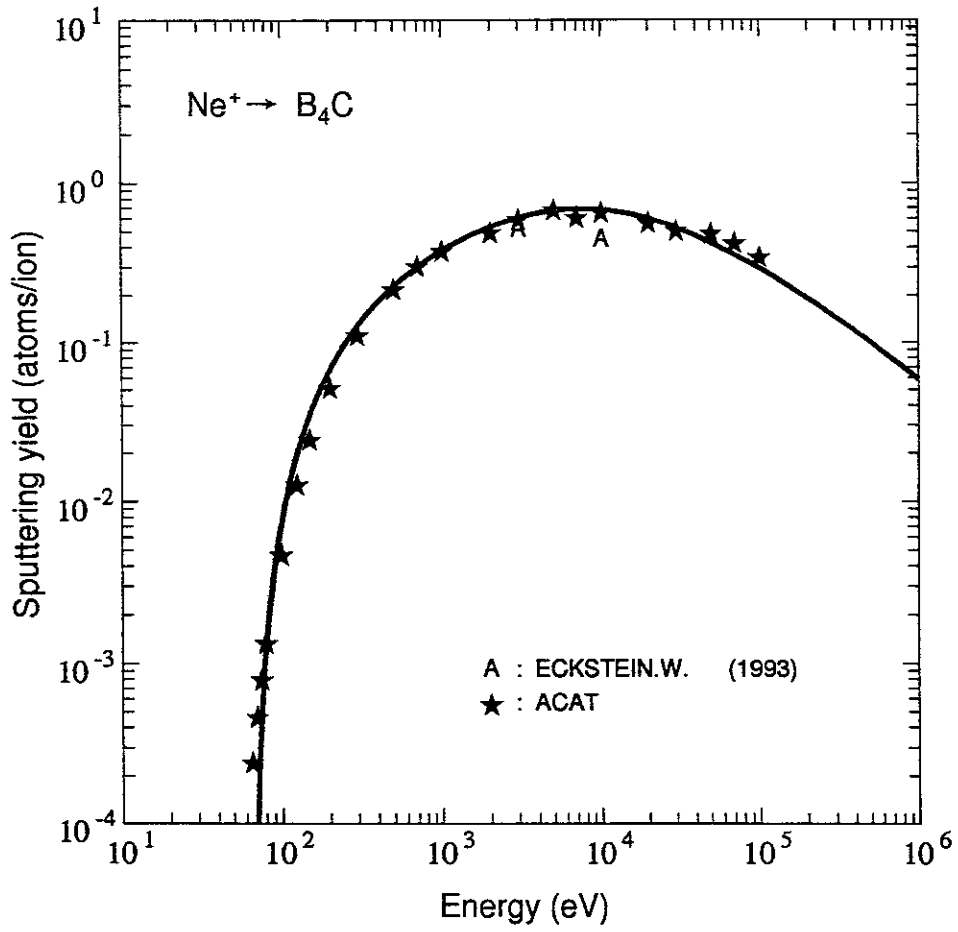


Fig. 7

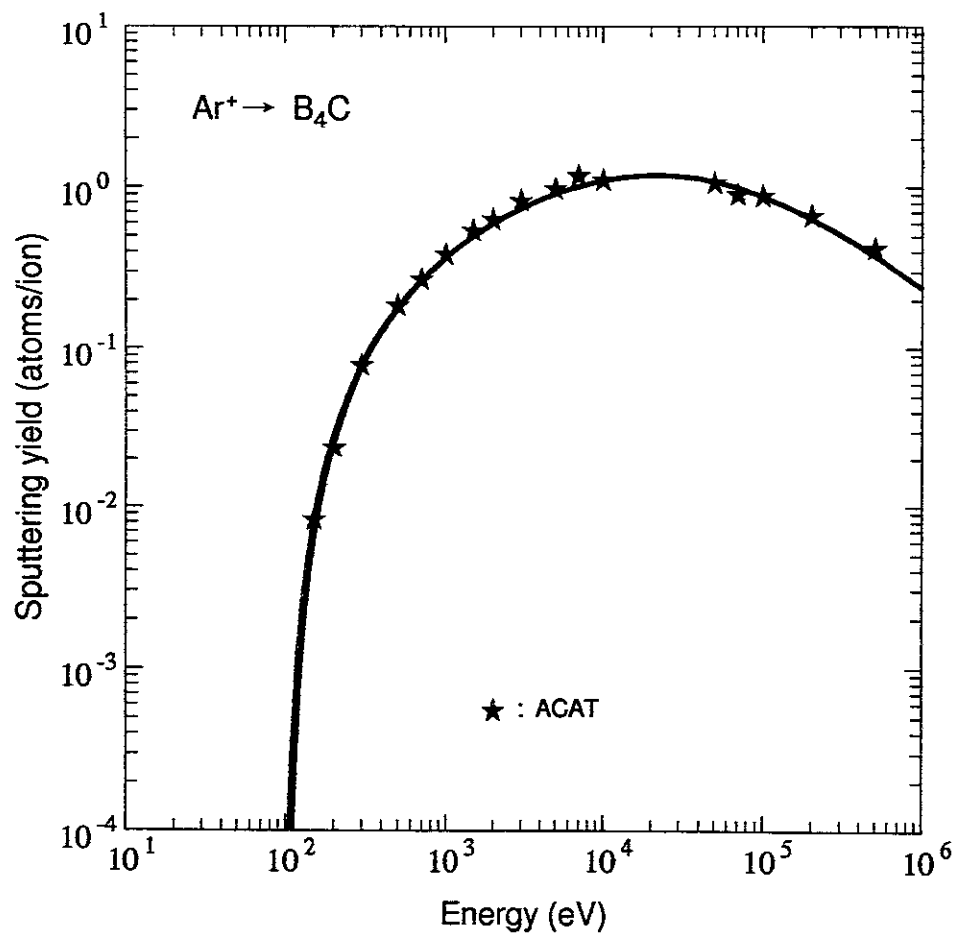


Fig. 8

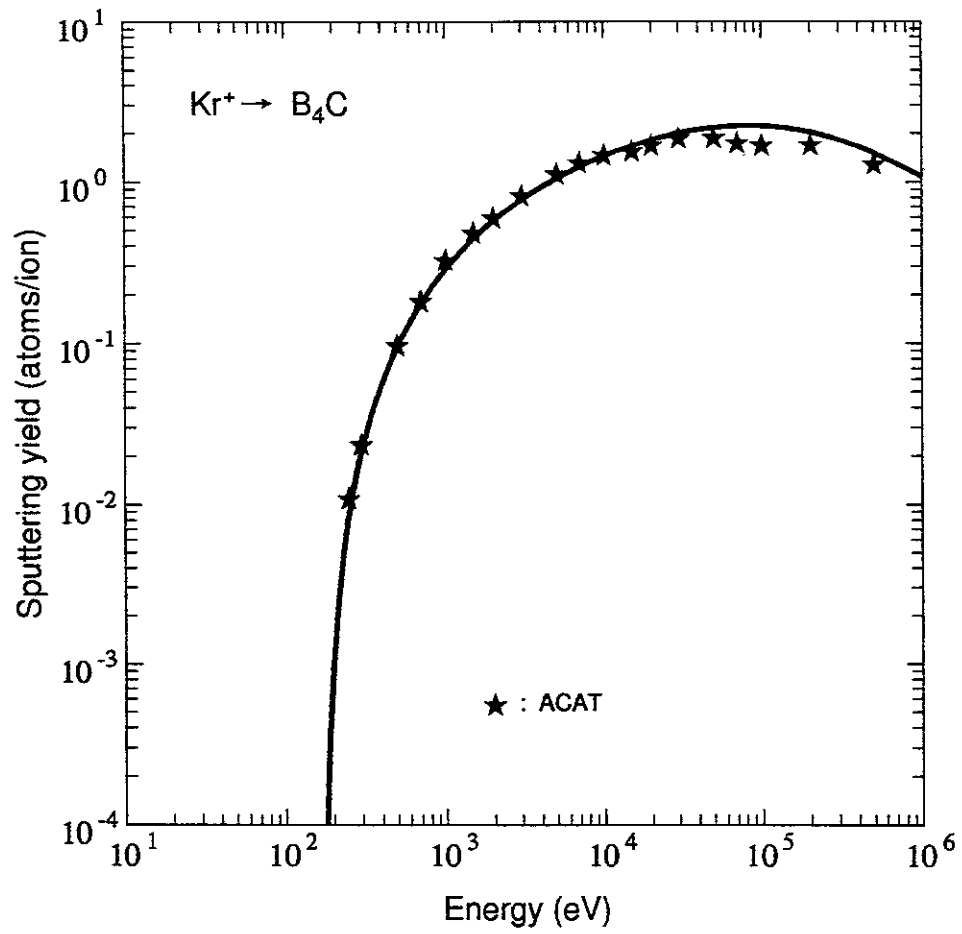


Fig. 9

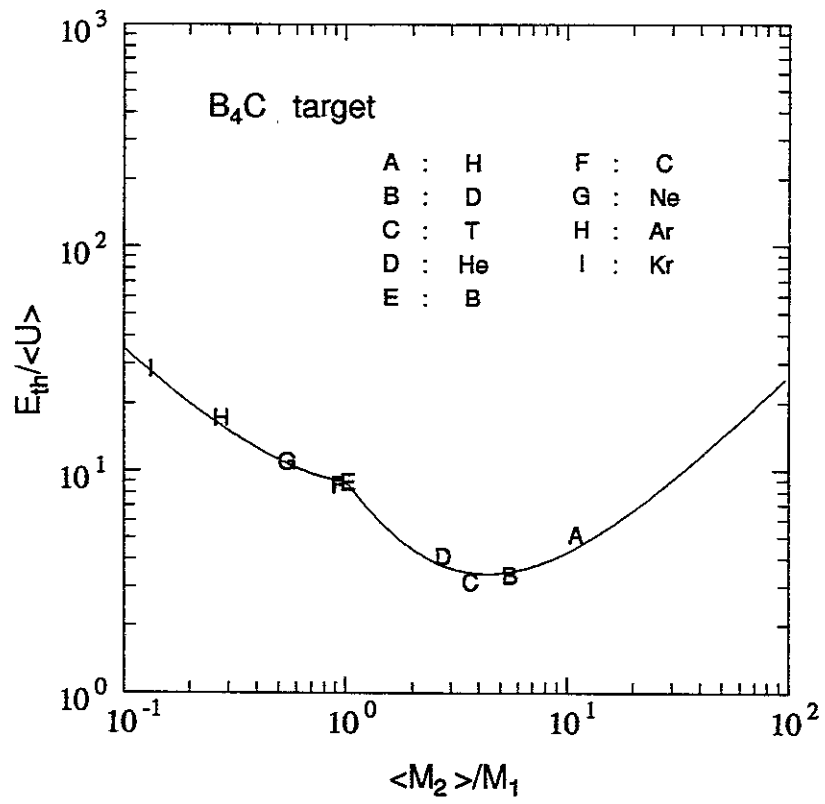


Fig. 10

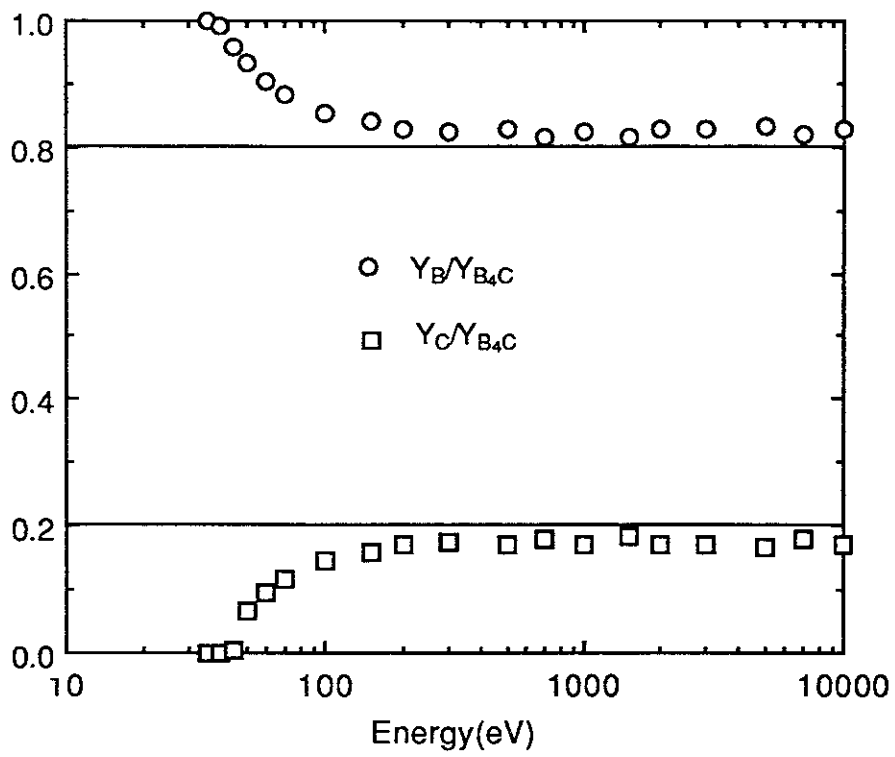


Fig. 11

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