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EVALUATION OF SOFT X-RAY AVERAGE RECOMBINATION COEFFICIENT AND AVERAGE CHARGE FOR METALLIC IMPURITIES IN BEAM-HEATED PLASMAS

By

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MAY 1986

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PREPARED FOR THE U.S. DEPARTMENT OF ENERGY,  
UNDER CONTRACT DE-AC02-76-CBO-3073.

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Printed in the United States of America

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EVALUATION OF SOFT X-RAY AVERAGE RECOMBINATION COEFFICIENT AND  
AVERAGE CHARGE FOR METALLIC IMPURITIES IN BEAM-HEATED PLASMAS

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ABSTRACT

The soft X-ray continuum radiation in TFTR low density neutral beam discharges can be much lower than its theoretical value obtained by assuming a corona equilibrium. This reduced continuum radiation is caused by an ionization equilibrium shift toward lower states, which strongly changes the value of the average recombination coefficient of metallic impurities  $\bar{\gamma}$ , even for only slight changes in the average charge,  $\bar{Z}$ . The primary agent for this shift is the charge exchange between the highly ionized impurity ions and the neutral hydrogen, rather than impurity transport, because the central density of the neutral hydrogen is strongly enhanced at lower plasma densities with intense beam injection. In the extreme case of low density, high neutral beam power TFTR operation (energetic ion mode) the reduction in  $\bar{\gamma}$  can be as much as one-half to two-thirds. We calculate the parametric dependence of  $\bar{\gamma}$  and  $\bar{Z}$  for Ti, Cr, Fe, and Ni impurities on neutral density (equivalent to beam power), electron temperature, and electron density. These values are obtained by using either a one-dimensional impurity transport code (MIST) or a zero-dimensional code with a finite particle confinement time. As an example, we show the variation of  $\bar{\gamma}$  and  $\bar{Z}$  in different TFTR discharges.

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## I. INTRODUCTION

Since the hot plasma in a fusion device interacts with a surrounding wall, one always finds this wall material as impurities in the plasma discharge. In most cases, at least part of the wall is metallic, so these metallic impurities are very often important ingredients of the plasma in addition to low-Z impurities such as oxygen and carbon. A large effort has gone into understanding different aspects of plasma impurities: radiation losses, influence on the stability of the discharge, influence on ignition for a fusion reactor, studies of new spectroscopic lines, and finally, the investigation of impurity transport. One particular question is the problem of the ionization balance for different impurities in the presence of different agents, which influence the transport, ionization, and recombination processes. The presence of neutral background, which can be either intrinsic, due to hydrogen sources at the walls, or extrinsic, as for neutral beam injection, can change this ionization equilibrium through the charge exchange process between the neutral hydrogen and highly ionized impurity. This effect is the strongest in the case of neutral beam injection into a low density plasma.<sup>1,2</sup> In this paper we describe the influence of this charge exchange process on the ionization equilibrium of medium-Z metals, the implications for recombination radiation, and the interpretation of soft X-ray spectra obtained by Pulse-Height-Analysis (PHA).

## II. IONIZATION EQUILIBRIUM IN THE PRESENCE OF CHARGE EXCHANGE

To obtain a charge state distribution for a particular impurity at any time in a discharge, one has to solve, in the most general case, a set of coupled continuity equations with proper initial and boundary conditions for a given plasma experiment. This set of coupled continuity equations in the case of cylindrical symmetry is given by<sup>3</sup>:

$$\frac{\partial n_i}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} r \Gamma_i = I_{i-1} n_{i-1} - (I_i + R_i) n_i + R_{i-1} n_{i-1} - \frac{n_i}{\tau_i} + S_i, \quad (1)$$

where subscript  $i$  denotes the ionization states,  $n_i$  is the impurity density in a charge state  $i$ ,  $I_i$  the ionization rate from ion  $i$  to ion  $(i+1)$ ,  $R_i$  the recombination rate from ion  $i$  to ion  $(i-1)$ ,  $\tau_i$  the volume loss time, and  $S_i$  the source and sink terms.  $\Gamma_i$  is the particle flux defined as

$$\Gamma_i = -D_i \frac{\partial n_i}{\partial r} + v_i n_i, \quad (2)$$

where  $D$  is a diffusion constant and  $v$  the convective velocity. The recombination rate contains several terms:

$$R_i = \alpha_i^{RR} n_e + \alpha_i^{DR} n_e + \alpha_i^{CX} n_0. \quad (3)$$

The first term is due to radiative recombination, and is specified by the radiative recombination rate coefficient  $\alpha_i^{RR}$ . The second term contains the dielectronic recombination rate coefficient,  $\alpha_i^{DR}$ . The last term is due to the charge exchange process between impurity ions and neutral hydrogen, and is determined by the charge exchange rate coefficient  $\alpha_i^{CX}$ . A special code (MIST) solves this set of coupled equations with one of the results being a charge state distribution for a given impurity.  $I_i$  and  $R_i$  are also functions of the electron temperature, so that the electron temperature and density profiles are fed into the code.

An even simpler numerical analysis is done with a zero-dimensional, steady-state code in which the transport and time derivative terms in Eq. (1) are dropped. Transport effects are simulated by an appropriate particle

confinement time  $\tau_i$ .<sup>4</sup> Because of its simplicity and reasonable accuracy for the center of the discharge where the PHA-observed emission is typically and predominantly emitted, most of the results were obtained using this code.

Both the MIST and the zero-dimensional code can utilize as inputs the electron temperature, electron density, and the neutral density and energy distribution from a TFTR diagnostic data analysis code (SNAP). This way, for each shot where SNAP results are available, one can obtain the corresponding charge state distribution for each impurity. The code also calculates related physical parameters: line radiation for different lines, radiation cooling, average recombination coefficients, average charges, etc.

In the case of high density ohmic plasmas, it is enough to consider the radiative and dielectronic recombination, because the central hydrogen neutral density in the discharge is normally very small. Particularly in the case of low density plasmas with neutral beam heating, however, the charge exchange recombination term can have a dominant effect on the charge state distribution, with the radiative and dielectronic processes as well as transport becoming relatively unimportant.

One such case -- a very strong perturbation of the ionization equilibrium for nickel impurity due to charge exchange between nickel ions and intrinsic and beam neutrals -- is the energetic ion mode in TFTR. The experimental parameters for this case are  $I_p = 800$  kA,  $B_t = 4.8$  T,  $a = 0.81$  m,  $R = 2.58$  m, the neutral beam injected power is 5 MW, and the peak electron temperature and density are 4.32 keV and  $2.03 \times 10^{13} \text{ cm}^{-3}$  respectively. We first used the zero-dimensional code without neutrals and to simulate the transport we made use of either  $\tau_i = 0.2$ s, which describes the central transport rather well, or  $\tau_i = \infty$ , which corresponds to corona equilibrium. The ionization equilibria in these two cases were almost identical. If we use the SNAP-code values for

neutral densities and energy distributions of the same discharge to interact with the plasma and the plasma impurities, one can then observe a very strong shift in ionization equilibrium toward the lower states due to charge exchange between the neutrals in the plasma and the nickel ions. The peak of the distribution shifted from the He-like ions toward the Li-like ions, and became much broader. The fully stripped nickel went down by two orders of magnitude and the H-like ion density decreased by a factor of 20. It is obvious that this effect changes very strongly the line radiation pattern and intensity, the continuum radiation, and the cooling rate of the medium-Z impurities in the plasma. Similar numerical studies have been performed for other medium-Z impurities (Ti, Cr, Fe) and all show the same effect. This perturbation in ionization equilibrium is pronounced particularly if the plasma density is low, so that the neutral beam can penetrate to the center of the discharge. In this situation, a high central neutral hydrogen to electron density ratio  $n_0/n_e$  is achieved by virtue of both a large  $n_0$  and small  $n_e$ .

### III. INFLUENCE OF CHARGE EXCHANGE ON AVERAGE RECOMBINATION COEFFICIENT AND AVERAGE CHARGE

The perturbation of the ionization equilibrium through a charge exchange with neutral hydrogen has a direct consequence in the interpretation of soft X-ray radiation. High resolution X-ray spectroscopy can observe directly the strong changes in the charge state distribution by observing the changes in the line intensities of the highly ionized medium-Z ions during neutral beam injection. The interpretation of the PHA spectra is more subtle because the spectral resolution is much poorer, and one cannot observe the changes in a particular charge state directly. The main observable change occurs in continuum radiation, with the total recombination radiation, summed over all

charge states, a function of the charge state distribution. The continuum radiation of a given impurity species is composed of bremsstrahlung or free-free radiation<sup>5</sup>

$$\frac{dP_{ff}}{dE} = 3 \times 10^{-15} \sum_i n_e n_i Z_{effi}^2 \bar{g}_{ff} \frac{\exp(-\frac{E}{kT_e})}{\sqrt{kT_e}} \quad (4)$$

and the recombination or free-bound radiation

$$\frac{dP_{fb}}{dE} = 3 \times 10^{-15} \sum_i n_e n_i (\gamma_i - 1) Z_i^2 \bar{g}_{fb} \frac{\exp(-\frac{E}{kT_e})}{\sqrt{kT_e}}, \quad (5)$$

where  $\gamma_i$  is the recombination coefficient for an ion of charge state  $i$  and is given by

$$\gamma_i = 1 + \frac{\bar{g}_{fb}}{\bar{g}_{ff}} \frac{Z_i^2}{Z_{effi}} \left\{ \frac{\xi}{n^3} \frac{\chi_i}{kT_e} \exp \frac{\chi_i}{kT_e} + \sum_{v=1}^{\infty} \frac{2\chi_H}{kT_e} \frac{Z_i^2}{(n+v)^3} \exp \left[ \frac{Z_i^2}{(n+v)^3} \frac{\chi_H}{kT_e} \right] \right\}. \quad (6)$$

Here  $n_e$  is electron density in  $\text{cm}^{-3}$ ,  $kT_e$  the electron temperature in keV,  $Z_i$  the ion charge in a charge state  $i$ ,  $E$  the photon energy in keV,  $\bar{g}_{ff}$  and  $\bar{g}_{fbi}$  the free-free and free-bound Gaunt factors, respectively,  $n$  the ground state,  $\xi$  the number of electron vacancies in shell  $n$ ,  $\chi_i$  the ground state ionization potential of the ion in charge state  $i$  in keV, and  $\chi_H$  the hydrogen ionization potential.

The total continuum radiation by a single impurity is the sum of bremsstrahlung and recombination radiation, and can be expressed by utilizing Eqs. (4) and (5) as

$$\frac{dP}{dE} = 3 \times 10^{-15} n_e n_z \bar{Z}^2 \bar{g}_{eff} \bar{\gamma} \frac{\exp(-\frac{E}{kT_e})}{\sqrt{kT_e}} \quad (7)$$

where

$$\bar{Z}^2 = \sum_i \frac{n_i}{n_z} Z_i^2 \quad (8)$$

is the average squared charge,

$$\bar{\gamma} = \sum_i \frac{n_i}{n_z} \gamma_i \quad (9)$$

is the average recombination coefficient, and  $n_z = \sum_i n_i$  is the total impurity density of the species Z. These two average values  $\bar{Z}$  and  $\bar{\gamma}$  are used in interpreting soft X-ray spectra. They have to be correctly evaluated for medium-Z impurities, otherwise the overall  $Z_{eff}$  value and the continuum-deduced low-Z impurity densities will be wrong.<sup>5</sup> As indicated in expressions (8) and (9) the average recombination coefficient  $\bar{\gamma}$  and the average charge  $\bar{Z}$  are functions of the charge state distribution  $n_i/n_z$ . Note also that  $\gamma_i$  from expression (6) is a function of  $kT_e$ . Since  $n_i/n_z$  depends very strongly on the neutral density  $n_0$  and electron temperature, we should expect  $\bar{\gamma}$  and  $\bar{Z}$  also to be functions of these. This is demonstrated in Figs. 1 and 2, where the dependence of  $\bar{\gamma}$  and  $\bar{Z}$  on neutral density and electron temperature is depicted for the given central electron density, beam energy, and transport term. These figures are obtained by using the zero-dimensional code. As the neutral density increases, the  $\bar{\gamma}$  value decreases from its almost corona equilibrium value, and at very high neutral densities approaches asymptotically the value of 1. At the same time the  $\bar{Z}$  value drops because the charge state distribution shifts more and more toward the lower charge states.

The influence of various plasma parameter regimes ( $n_e$ ,  $P_b$ ,  $kT_e$ ) on  $\bar{\gamma}$  is shown in Fig. 3. Each point represents one TFTR discharge at the time of SNAP-code calculations (Thomson scattering time). The data points were obtained again by using a zero-dimensional code and were occasionally checked by the MIST code. The black symbols represent the "energetic ion" discharges, characterized by low electron density, high beam power, and high  $q$ . All these  $\bar{\gamma}_{Ni}$  are by more than a factor of two lower than the corresponding corona equilibrium values. In these cases the average charge  $\bar{Z}$  is decreased by more than one from the corona equilibrium  $\bar{Z}$ . On the other hand, in the case of medium and high density discharges (open points), even if the beam power is high, we observe just a small decrease of  $\bar{\gamma}_{Ni}$  from its corona equilibrium value. For these discharges the decrease in  $\bar{Z}$  is almost imperceptible. In almost all "black symbol" discharges, if the lowering of the medium-Z  $\bar{\gamma}$ 's due to charge exchange is not taken into account, but the  $\bar{\gamma}$ 's and  $\bar{Z}$ 's are assumed to be mainly given by the transport and the radiative and dielectronic rates, we observe that the measured continuum is lower than the evaluated recombination radiation due to medium-Z impurities, which then in the PHA analysis code produces negative carbon and oxygen densities. By "reinstating" the charge exchange effects, these difficulties disappear and the PHA code gives reasonable values for the carbon and oxygen densities.

#### IV. SUMMARY AND CONCLUSIONS

The combination of low density and neutral beam injection can perturb the ionization equilibrium of medium-Z impurities very strongly. In the extreme case of the "energetic ion" discharge in TFTR, the charge exchange processes between the highly ionized medium-Z ions and hydrogen neutrals completely dominate the establishment of the central ionization equilibrium over normal

recombination processes and transport. The charge state distribution is very much shifted toward the lower charge states. This, in turn, has a profound effect on the pattern of line radiation, recombination radiation, radiation cooling, and the interpretation of the soft X-ray PHA spectra. The TFTR energetic ion discharges show a decrease in medium-Z recombination radiation by more than a factor of two as a consequence of charge exchange. The charge exchange processes with low-Z impurities do not influence the recombination radiation in the soft X-ray region very much because the low-Z impurities are mostly in a fully stripped state in the center of the discharge, although they significantly alter the line radiation intensities.

#### ACKNOWLEDGMENTS

This work was supported by U.S. Department of Energy Contract No. DE-AC02-76-CH0-3073.

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## FIGURE CAPTIONS

Fig. 1. Dependence of the nickel average recombination coefficient on the beam neutral density and electron temperature. The energy of beam neutrals is 80 keV,  $\tau_p = 0.2$  s and  $n_e = 3 \times 10^{13} \text{ cm}^{-3}$ .

Fig. 2. Dependence of the nickel average charge on the beam neutral density and electron temperature. The other parameters are the same as in Fig. 1.

Fig. 3. Variation of the nickel average recombination coefficient with electron temperature, electron density, and beam energy. The black symbols represent the "energetic ion" discharges. The solid line is the corona equilibrium case.

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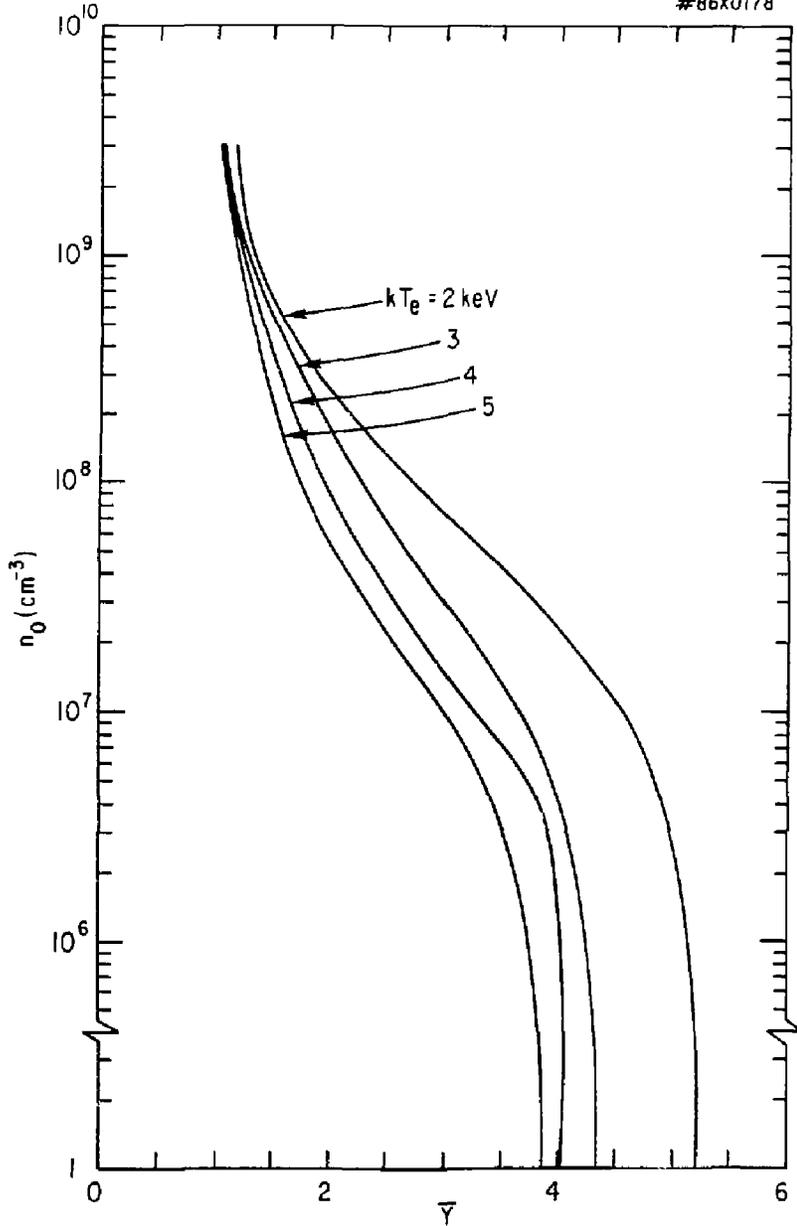


Fig. 1

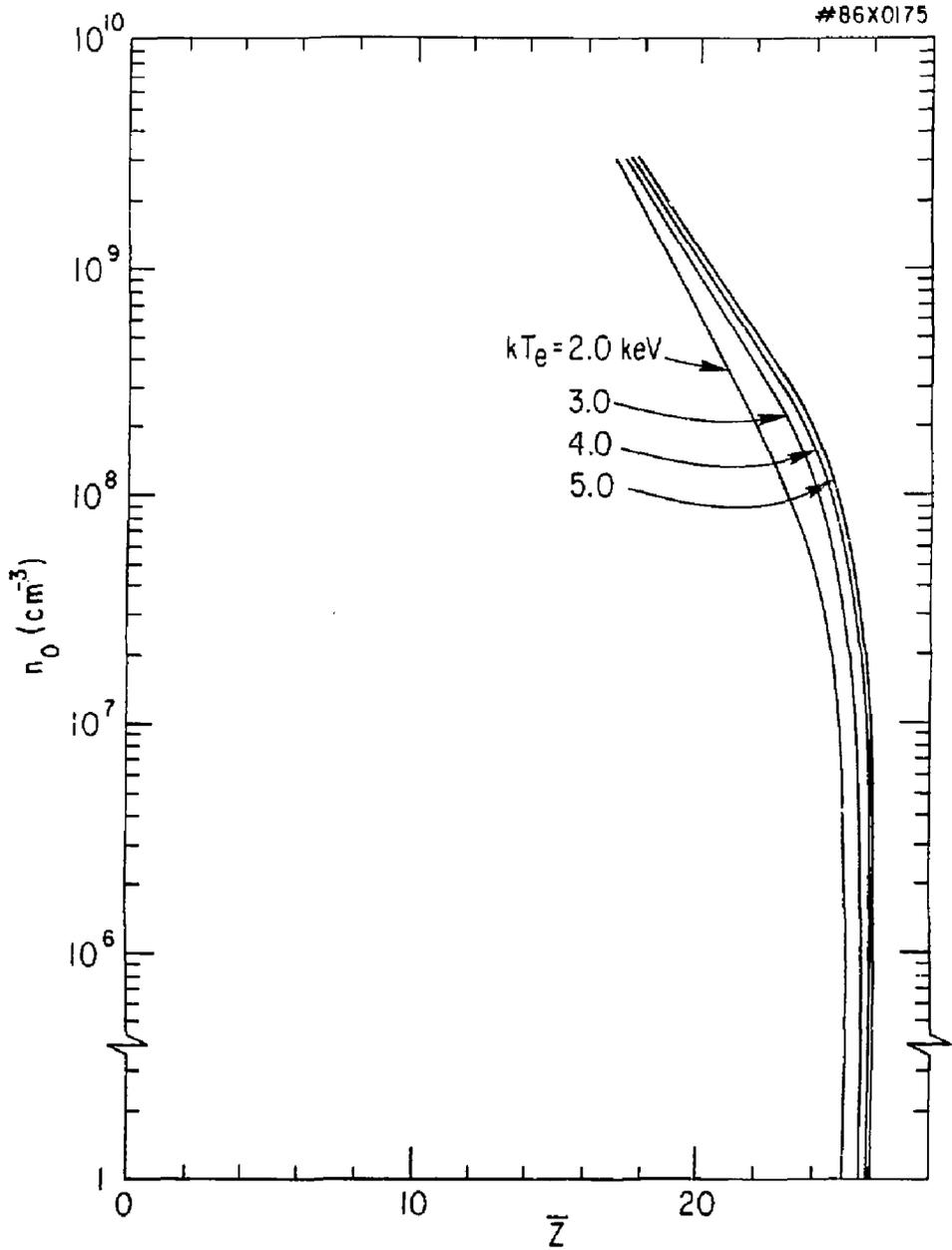


Fig. 2

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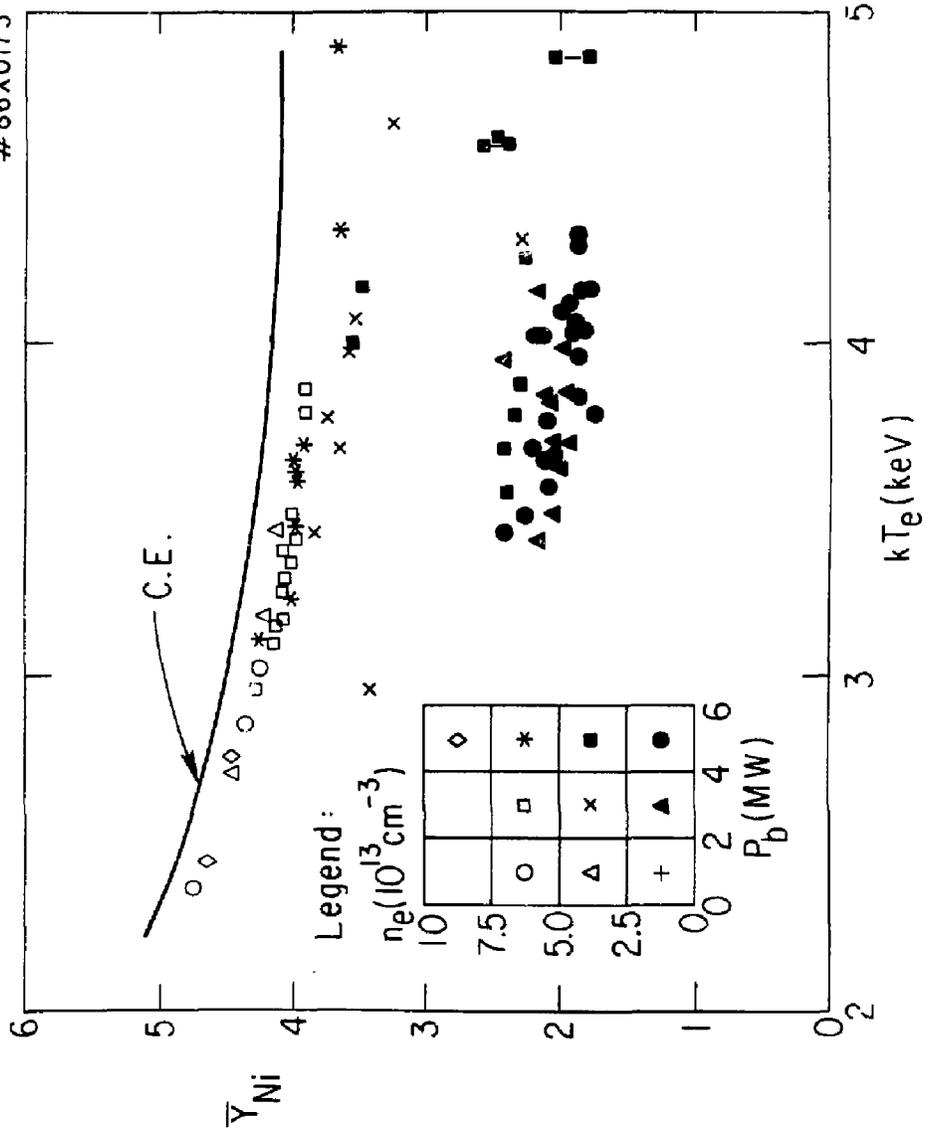


Fig. 3

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