DEPOLARIZATION OF D-T PLASMAS BY RECYCLING IN MATERIAL WALLS

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ABSTRACT

The feasibility of using polarized deuterium (D) and tritium (T) plasmas in fusion reactors may be seriously affected by recycling in material walls. Theoretical and experimental results are reviewed which show how the depolarization rates of absorbed D and T depend on first wall parameters such as the temperature, the bulk and surface diffusivities, the density of electronic states at the Fermi surface, the spectral density of microscopic fluctuating electric field gradients, and the concentration of paramagnetic impurities. Nuclear magnetic resonance (NMR) spectroscopy of hydrogenated and deuterated amorphous semiconductors suggests that low-Z nonmetallic materials may provide a satisfactory first wall or limiter coating under reactor conditions with characteristic depolarization times of several seconds. Experiments are proposed to test the consequences of our analysis.

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1. INTRODUCTION

Kulsrud, Furth, Valeo, and Goldhaber recently suggested that the performance of magnetic confinement fusion reactors could be improved by using polarized deuterium and tritium (D-T) plasmas.¹ By polarizing the plasma ions, one can enhance or suppress nuclear fusion rates and control the angular distribution of emitted reaction products. For example, if all nuclei are polarized to have parallel magnetic dipole moments, the D-T fusion cross section is increased 50%. This enhancement would allow engineers to use a 10% weaker magnetic field or a 20% smaller β (ratio of particle pressure to magnetic pressure) to achieve the same power output as that obtained with an unpolarized plasma.² If the D nuclei are polarized orthogonally to $\vec{B}$ (the confining magnetic field), the neutron loading of the walls may be reduced.³

The feasibility of using polarized plasmas depends on a technology that can create and inject large quantities of polarized D and T. It also depends on the absence of physical mechanisms that can depolarize the plasma rapidly on the time scales of particle confinement (~ 1 sec) or fuel burnup (~ 100 sec). Recent advances in the physics of optical pumping⁴ and in the study of spin-aligned atomic hydrogen⁵ seem to provide solutions for the first problem; their practical implementation is currently underway. A major contribution of Kulsrud et al. was to show that the second problem also seems to be solved; the obvious depolarization mechanisms in the plasma are too weak to be relevant. These two advances are the main impetus for considering plasma polarization in future reactors.

There are, however, other depolarization mechanisms present which have not been considered carefully, and which are more important than those occurring in the plasma. These arise from the recycling of D and T at the limiter and the first wall of the reactor vessel (Fig. 1). In all magnetic

confinement schemes studied to date, the D-T fuel leaks out across the magnetic field lines about 10 to 20 times faster than the rate of fuel consumption.⁶ (Indeed, for a burning plasma, the ions must leak out at an appreciable rate in order for the helium ash to leave the plasma core.) As a consequence, most particles leave the plasma, strike the limiter (or first wall) and reenter the plasma about 20 times before fusing or before being pumped away. About half the flux of particles striking the first wall is reflected back into the plasma.⁷ The remaining particles have sufficient kinetic energy (20-100 eV) to penetrate about 100 Å into the wall.⁸ There the D and T ions come to equilibrium and eventually diffuse back to the surface where they recombine and desorb as molecules, or are desorbed directly by ion, electron, and photon bombardment.

The D and T nuclei in the crystal lattice and in the vicinity of the wall surface are subject to depolarization mechanisms that are not present in the plasma core. In the plasma edge and in cracks or voids of the wall material, D and T can exist as polyatomic molecules. For these species, tumbling caused by collisions between of the molecules can flip the nuclear spins. For absorbed D and T residing in the crystalline lattice, depolarization can occur by thermal diffusion and by phonon and electron induced fluctuations of microscopic magnetic fields and electric field gradients (which couple to nuclear magnetic dipole and electric quadrupole moments, respectively).

These new mechanisms can greatly reduce the nuclear magnetization of D and T on time scales of 10^{-3} to 10^1 seconds. Since the mean residence time of absorbed D and T in the wall is also comparable with these time scales, a careful choice of the composition and temperature of the first wall and limiter is crucial in preventing rapid depolarization of the plasma.

In this paper, we review and analyze theoretical and experimental results

which show how the D and T depolarization rates depend on the material properties and temperature of the first wall. Our goal is to introduce the relevant theory and literature to plasma physicists and to stimulate research on low-Z wall materials and coatings that will have good mechanical durability and slow depolarization rates. Our discussion suggests that nonmetallic materials, especially hydrogenated amorphous semiconductors, may provide a satisfactory first wall or limiter coating under reactor conditions. Our analysis also points out important gaps in our knowledge which prevent us from making quantitative estimates of depolarization rates. Especially important is whether there will be large surface concentrations of paramagnetic impurities. Finally, we suggest future experiments which can test whether all the important theoretical elements have been anticipated and correctly understood. These experiments are useful in their own right since they also measure quantities of direct importance for the design of first walls, such as diffusivities and residence times.

An accurate estimate of the depolarization rate for plausible wall materials under reactor conditions is difficult at present. The reasons are fourfold. First, theoretical calculations depend sensitively on features of the electronic structure such as the density of electronic states at the Fermi surface⁹ (for metals) and the spectral density of electric field gradient fluctuations at interstitial sites.¹⁰ These features are hard to calculate even for the simplest crystal structures. Second, many depolarization mechanisms depend on thermally activated processes such as diffusion, and capture and release by traps. The exponential dependence of these processes on barrier energies and reciprocal temperature makes quantitative estimates difficult. Third, while nuclear magnetic resonance (NMR) techniques routinely provide information about absorbed D and T depolarization rates,¹¹ most

experiments to date have studied highly purified and homogeneous samples. These experiments are unlikely to be relevant since the energetic processes occurring at the first wall rapidly disorder the crystal lattice, introducing a variety of defects and impurities. The chemical and physical properties of the outermost layer of first wall and limiter have not yet been well characterized, especially during reactor conditions.

Finally, even with a thorough understanding of the possible depolarization mechanisms, the depolarization rate is hard to estimate because it depends on how long the implanted ions reside in the wall before returning to the plasma. This residence time (of order 10^{-3} to 10^1 sec) is governed by the evolving bulk concentration profile of D and T which, in turn, depends on the flux rate, wall material, temperature gradient, and surface desorption processes. (The surface is particularly hard to control since there is likely to be constant erosion and redeposition of the outermost wall layer.) The profile also depends on engineering designs which determine the wall tritium inventory, e.g., by not allowing permeation of tritium through the first wall and into the reactor coolant. A discussion of residence times and their measurements for candidate wall materials is complex and will not be given here; reviews of recent experiments can be found in the literature.¹²

The remaining part of the paper is organized as follows. In Sec. 2, we briefly review the physics of NMR spectroscopy, especially the concepts of T_1 and T_2 . This provides a useful context for understanding the various depolarization mechanisms as well as for interpreting the experimental data. In Secs. 3 and 4, we discuss depolarization mechanisms of the edge, bulk, and surface regions, respectively. The processes of the latter two regions are closely related and are conveniently discussed together. Finally, in Sec. 5, we summarize our discussion and suggest some future experiments.

2. NUCLEAR MAGNETIC RESONANCE AND DEPOLARIZATION RATES

The polarized nuclei in the walls constitute an ensemble of particles which are weakly coupled to external degrees of freedom (the "lattice") and to each other. The two kinds of couplings introduce two different macroscopic time scales, called the longitudinal and transverse relaxation times in the NMR literature.¹³ These are denoted by T_1 and T_2 , respectively. In this section, we discuss how the depolarization rates of D and T depend on T_1 and T_2 . We also discuss the microscopic processes and time scales which determine the magnitude of T_1 .

If the ensemble of nuclei is not in thermal equilibrium with the surrounding lattice, energy is exchanged with the lattice until the occupation of each nuclear state is proportional to its Boltzmann factor, $\exp(-E_m/k_B T)$. Here E_m is the energy of a particular nuclear state, k_B is the Boltzmann constant, and T is the absolute temperature of the lattice. For typical nuclear magnetic dipole moments $\vec{\mu}$ (of order 10^{-24} ergs G⁻¹), in the presence of typical reactor fields $\vec{B} = B_0 \hat{z}$ ($B_0 \sim 10^5$ G), the equilibrium nuclear magnetization, which is proportional to $\tanh(\mu B_0/k_B T)$, is vanishingly small for $T \gtrsim \mu B_0/k_B \sim 10^{-3}$ K. Thus for typical wall temperatures ($T \gtrsim 300$ K for the wall, 1000 K for the limiter) polarized nuclei will relax to a zero equilibrium magnetization by exchanging energy with the lattice. This decay of nuclear magnetization often occurs exponentially over a time scale which is defined to be T_1 , the longitudinal relaxation time. The depolarization rate of nuclei is then simply T_1^{-1} .

The coupling of nuclear spins to one another in the absence of the lattice determines the second macroscopic time scale, T_2 . This is the characteristic time for information about spin orientation to diffuse to different members of the ensemble, e.g., by repeated mutual spin flips.

Nuclear depolarization rates can depend on T_2 when the depolarization mechanisms are not spatially homogeneous, e.g., in the case of isolated paramagnetic impurities (see Sec. V). At lower temperatures, when atomic diffusion can be ignored, T_1 then depends on the rate at which spin diffusion¹⁴ carries the nuclear magnetization towards the depolarizing centers.

Spin diffusion and T_2 do not play a role in wall depolarization. Reactor wall temperatures are so high that atomic diffusion will always transport nuclear magnetization more rapidly than spin diffusion. Furthermore, in a wall containing equal concentrations of D and T, energy-conserving spin flips are inhibited since nearest neighbor nuclei are likely to have different nuclear magnetic dipole moments.

T_1 (and T_2) can be easily measured by numerous NMR techniques, and has been measured for many hydrogen and deuterium containing substances. Its order of magnitude is determined by the relative size of two microscopic time scales, the inverse Larmor frequency ω_0^{-1} ($\omega_0 = \gamma B_0 \sim 10^9 \text{ sec}^{-1}$ where γ is the nuclear gyromagnetic ratio, see Table 1) and the correlation time, τ_c , of microscopic fluctuations in the magnetic field or electric field gradients. The depolarization rate is a maximum (for fixed ω_0 , i.e. fixed external field) when these two time scales are comparable

$$\omega_0 \tau_c \approx 1. \quad (1)$$

Thus the temperature and composition of the walls should be chosen so that Eq. (1) is not satisfied by any depolarization mechanism. This, as we will see, requires nonmetallic walls at high temperatures in which case $\omega_0 \tau_c \ll 1$.

This qualitative result [Eq. (1)] is confirmed by quantum mechanical

calculations of transition rates caused by a random time-dependent perturbation. If the autocorrelation matrix of the components of the microscopic magnetic field is isotropic (equal diagonal elements, zero off-diagonal elements), and decays exponentially over a correlation time, τ_c , it can be shown that T_1 is given by

$$T_1^{-1} = \gamma^2 \langle b_L^2 \rangle \frac{2\tau_c}{1 + \omega_0^2 \tau_c^2} \quad (2)$$

where γ is the gyromagnetic ratio of the nucleus, and $\langle b_L^2 \rangle$ is the mean square amplitude averaged over time of the microscopic magnetic fields. (We have ignored a similar term at frequency $2\omega_0$.) This formula - first derived and tested by Bloembergen, Purcell, and Pound (abbreviated BPP)¹⁵ - is valid for random motion of nuclei in gases and liquids. It is also valid for nuclei in solids when the nuclei are mobile, i.e., there is thermal diffusion. The BPP formula relates the macroscopic depolarization rate, T_1^{-1} , to the microscopic time scales ω_0^{-1} and τ_c .

Different relaxation mechanisms have their own characteristic correlation times, τ_c . The measured depolarization rate will then be a sum of individual rates

$$(T_1^{-1})_{\text{total}} = T_{11}^{-1} + T_{12}^{-1} + \dots, \quad (3)$$

where each T_{11}^{-1} has the BPP form, Eq. (2).

The discussion so far has emphasized the interaction of nuclear magnetic dipole moments with the confining magnetic field, $\vec{B}$. The deuteron also has a small electric quadrupole moment (as do many nuclei with $I > 1/2$) which can interact with microscopic electric field gradients. Such gradients arise from

asymmetric crystalline environments such as noncubic lattice sites, surfaces, and lattice defects. They also arise from anisotropies in electron charge densities, e.g., p-valence electrons in a covalent bond. These gradients typically have magnitudes at most of e/a^3 where a is roughly a lattice constant (10^{-8} cm).

The electric field gradient tensor has a time dependence because of lattice vibrations (phonons). This time dependence can induce quadrupole transitions which change the orientation of the nuclear quadrupole moment with respect to the local electric field gradients. This in turn changes the orientation of the magnetic dipole moment (which is rigidly oriented with respect to the electric quadrupole), providing another relaxation mechanism. The contribution to the depolarization rate, Eq. (3), again has the form Eq. (2) except that the magnetic interaction energy $\gamma^2 \langle b_L^2 \rangle = (\mu B_0 / \hbar)^2$ is replaced by (ignoring numerical prefactors of order 1)

$$\left(1 + \frac{\eta}{3}\right) \left[\frac{eQV_{33}}{\hbar} \right]^2, \quad (4)$$

where Q is the electric quadrupole moment in cm^2 ,

$$\eta = \frac{V_{11} - V_{22}}{V_{33}} \quad (5)$$

is an asymmetry parameter (between 0 and 1) and $V_{33} > V_{22} > V_{11}$ are the principle eigenvalues of the local electric field gradient tensor.

The electric quadrupole interaction energy is frequently larger than the interaction energies of fluctuating microscopic magnetic fields. The dominant depolarization mechanism for deuterons is therefore phonon modulated quadrupole transitions.

We can summarize this section as follows. The depolarization rate of nuclei is given by T_1^{-1} where T_1 , the longitudinal relaxation time, is easily measured by NMR spectroscopy. The depolarization rate depends on T_2 , the transverse relaxation time, only at temperatures which are so low that atomic diffusion of the nuclei can be ignored. T_1 depends on two microscopic time scales, the inverse Larmor frequency, ω_0^{-1} , and the correlation time, τ_c . The depolarization rate obeys the BPP formula, Eq. (2), if the microscopic fluctuations are exponentially correlated with a correlation time τ_c ; the rate reaches a maximum for fixed ω_0 when Eq. (1) is satisfied. Transitions which repopulate the nuclear quantum levels and depolarize the nuclei are induced by nuclear motion which modulates the nuclear magnetic dipole moment. The deuteron also can depolarize by modulation of its electric quadrupole moment, which is usually its dominant relaxation process.

3. PLASMA EDGE DEPOLARIZATION

The plasma edge is a transition region near the walls, typically 10-20 cm in radial extent, where the large densities and temperatures of the plasma core decrease to their small values at the wall. The partially ionized plasma of the edge contains charged and neutral species (e.g., e^- , D, D^+ , T, T^+ , D_2 , T_2 , DT, DT^+ , D_3^+ , T_3^+ , etc.) which interact with each other. The densities of these species is typically of order 10^{10} to 10^{13} cm $^{-3}$.

Most depolarization mechanisms in the edge are the same as those discussed by Kulsrud et al. for depolarization in the plasma core. Even when the slower velocities and longer collision times are taken into account, collisions by Coulombic, spin-orbit, spin-spin, and quadrupole interaction are too inefficient ($T_1 \gtrsim 10^5$ sec) to give significant depolarization. Processes in the cooler edge such as charge exchange or recombination of nuclei with

electrons of opposite spin do not lead to depolarization because the magnetic field is large. The probability of the admixed atomic state with the nucleus reversed is proportional to $(B_c/B_0)^2$ where $B_c \sim 10^3$ G (for hydrogen) is the critical field for which the Zeeman and hyperfine splittings are equal.¹⁶ For reactor fields $B_0 \sim 10^5$ G, and the electron magnetic moment is nearly decoupled from the nucleus.

The most dangerous depolarization mechanism in the plasma edge occurs for nuclei of diatomic and triatomic species such as L_2 , NT^+ , D_2T^+ , etc., which are free to tumble. These nuclei can relax by random rotations which modulate the dipole-dipole interaction and by interaction with the magnetic dipole moment formed by rotation of the molecular electron cloud. The Hamiltonian can be written as¹⁷

$$H_{\text{int}} = \gamma \{ H' (\vec{I}_1 + \vec{I}_2) \cdot \vec{J} + 2H'' (\vec{I}_1 \cdot \vec{I}_2 - 3(\vec{I}_1 \cdot \hat{n})(\vec{I}_2 \cdot \hat{n})) \} , \quad (6)$$

where γ is the nuclear gyromagnetic ratio (Table I), $\vec{I}_1$ and $\vec{I}_2$ are the spin vectors of the two nuclei. $\vec{J}$ is the molecular rotational angular momentum, and $\hat{n}$ is the unit vector pointing between nuclei. The effective field strengths H' and H'' are known from molecular beam experiments and are given by¹⁸

$$H' = 27 \text{ G} ; \quad H'' = 34 \text{ G} .$$

The two contributions to Eq. (6) therefore have comparable magnitudes. In the following, we consider only the spin-rotation coupling; the total relaxation rate will be roughly three times our estimated value.

A calculation shows that the longitudinal spin-rotation depolarization rate is given by¹⁹

$$T_1^{-1} = \frac{2}{3} J(J+1)(\gamma H')^2 \frac{\tau_c}{1 + (\omega_J - \omega_0)^2 \tau_c^2} \quad (7)$$

where J is the quantum rotation number (usually 1 for the lowest excited rotation state), $\omega_J = \gamma_J B_0$ is the Larmor frequency of the rotation-induced molecular magnetic moment ($\gamma_J \approx 3.9 \times 10^3 \text{ G}^{-1} \text{ sec}^{-1}$ for H_2), and τ_c is a correlation time.

In a gas consisting only of identical diatomic molecules, say H_2 , τ_c would simply be the collision time (actually, the collision time for disorientation of the molecular rotation axis, which can be longer than the usual kinetic collision time). In the plasma edge, collisions are just as likely to destroy the molecule or change its charge state as well as to disorient it. Thus τ_c^{-1} must be determined as a sum, $\sum n_i \sigma_i \bar{v}_i$, over the densities, cross sections, and relative velocities of each process (ionization, dissociation, etc.) that can change the magnetic field felt by the nuclei of the diatomic molecule. Experimental data²⁰ show that the smallest τ_c is of order 10^{-7} sec, with typical values of $10^{-7} < \tau_c < 10^{-4}$ sec. For diatomic hydrogen (for which we can assume $J = 1$, $\tau_c = 10^{-7}$ sec, $B_0 = 10^5 \text{ G}$, $H' = 27 \text{ G}$, $\gamma = 2.7 \times 10^4 \text{ G}^{-1} \text{ sec}^{-1}$), Eq. (7) gives a depolarization rate of $T_1^{-1} \sim 1.0 \text{ sec}^{-1}$. This is much faster than any of the processes considered by Kulsrud et al. It is, however, very small compared to the inverse correlation time. Most diatomic molecules will break up long before the nuclei can depolarize.

The above estimate was for a neutral homonuclear molecule. Charged molecules such as T_2^+ and D_2^+ have even smaller relaxation rates since the rotational magnetic moment is smaller (lower electronic charge density and larger moment of inertia) and the nuclei are further apart (e.g., the

equilibrium bond length of H_2^+ is 0.3 Å larger than that of H_2^{21}). Heteronuclear molecules such as DT and $(DT)^+$ have a weaker dipole-dipole interaction. Also, relaxation by the hyperfine interaction of the unpaired electron¹ of these charged species is suppressed by the strong external magnetic field. Thus depolarization is slower for the other diatomic species. Similar arguments can be made for the triatomic molecules. The plasma edge is therefore an insignificant source of nuclear depolarization.

Before concluding this section, we note that the spin-rotation process which dominates the depolarization mechanisms of the plasma edge can also occur in cracks or voids of the wall material. On the surfaces of such interior volumes, nuclei can recombine into diatomic form, tumble, and depolarize. Unlike the plasma edge, there are no collisions, except with the surface, which can break up the molecule before depolarization occurs; the situation is potentially more serious. The contribution of this process to the total depolarization rate will depend on the rate of collisions [τ_c in Eq. (7)], the fraction of D and T in such voids, and the rate at which bulk nuclei exchange with nuclei in the gas phase, a highly surface and material dependent number. Spin-rotation may therefore be important in materials in which hydrogen or helium is weakly soluble, leading to blistering and cracking under high flux rates. This suggests an obvious criterion for first wall and limiter materials. It would be useful to study the importance of this effect directly by measuring the depolarization rate as a function of temperature and porosity, e.g., in zeolites whose interior volumes can be made uniform and of different sizes.²²

Finally, we point out that the molecular magnetic moment is strongly coupled to the lattice for diatomic species that are bound to the surfaces of cracks and voids. Nearby diffusing nuclei, which are not part of the diatomic

molecule, become coupled to the lattice in the vicinity of these molecules and can rapidly depolarize. (See Sec. 4C where we discuss such paramagnetic interactions.) This relaxation mechanism has been suggested²³ to be the dominant one for both D and T in hydrogenated amorphous semiconductors below 300°C and is likely to play a role in the depolarization of plasmas by nonmetallic walls.

4. BULK AND SURFACE DEPOLARIZATION

The relaxation mechanisms of the bulk and surface regions of the limiter and first wall are closely related and are best discussed together. There are three important mechanisms which we discuss in turn: hyperfine coupling of nuclei to unbound (conduction) electrons, dipole-dipole interactions modulated by atomic diffusion, and interactions with paramagnetic impurities (unpaired bound electrons). Of course, there are many other processes such as surface desorption, phonon modulation of magnetic dipole moments, etc. These are either weaker than the ones we discuss or can be estimated from our discussion.

A. Depolarization by conduction electrons

Longitudinal relaxation of nuclei involves transitions which require the emission or absorption of a quantum of energy $\hbar\omega_0 = \mu B_0 \sim 10^{-7}$ eV. The lattice is fundamentally different from atomic or molecular systems in having a continuum of quantum levels to which this small but finite energy can be transferred or withdrawn. In particular, metals are characterized by a continuum of electronic states whose occupations are governed by the Fermi-Dirac distribution. In momentum space, all states are occupied up to the Fermi energy, E_F , above which there are infinitesimally nearby unoccupied

states. An electron at the Fermi level can inelastically scatter and spin-flip a nucleus, carrying the small spin-flip energy as an increase in its kinetic energy to a nearby quantum level above the Fermi surface. At finite temperatures, only a small fraction of electrons near the Fermi surface (of order $k_B T/E_F$ where T is the lattice temperature and the Fermi energy is typically about 5 eV) can inelastically scatter. This suggests that the depolarization rate is proportional to the temperature.

A detailed calculation confirms this.²⁴ The electronic longitudinal relaxation time, T_{1e} , may be written in the form:

$$T_{1e} T = K, \quad (8)$$

the so-called Korringa relation. The constant K is independent of the temperature T and the external magnetic field strength, B_0 ; it contains powers of the electronic magnetic susceptibility and of the density of electronic states at the Fermi level,⁹ both of which are hard to calculate from first principles. Values of K for metallic hydrides have been measured and are typically 50-500 sec K in magnitude.¹¹ Thus relaxation times of order 0.1 sec or smaller can be expected (and are observed).

The electron depolarization rate increases with increasing temperature. Because of the large velocity of electrons at the Fermi level [of order $(2E_F/m_e)^{1/2} \approx 10^8$ cm/sec], the depolarization rate is also independent of the slow diffusive motion of nuclei at higher temperatures. Since a high temperature is needed to minimize the depolarization rates discussed below, we conclude that first wall materials should be nonmetallic to prevent significant plasma depolarization. More precisely, wall materials should have a small or vanishing density of s- and d-electron states at the Fermi

surface.⁹ A semimetal such as graphite has a small (lower-dimensional) Fermi surface and may give acceptable D and T electronic relaxation rates, as suggested by spin-lattice relaxation measurements²⁵ of ^{13}C nuclei.

The requirement for the Korringa relation to hold is that there are unbound electrons with nearby unoccupied electronic levels (in momentum space) of slightly higher energy. On metallic surfaces, hydrogen (D and T) forms strong localized covalent bonds with nearby metal atoms.⁹ The Pauli exclusion principle then leads to a reduced projected density of conduction electron states on the surface hydrogen. A longer relaxation time, T_{1e} , is therefore predicted. Recent experiments by Slichter and collaborators indeed confirm that the Korringa relaxation rate decreases from the bulk to the surface, nearly vanishing for the latter.²⁶ Thus hydrogen-covered metal surfaces will not be strong sources of depolarization. This assumes the absence of an appreciable surface concentration of paramagnetic impurities, as we discuss further below.

A simple consequence is that a metal surface weakly depolarizes the reflected D and T ions; most collisions occur within the first few surface layers, for which the Korringa relaxation rate should be small. Since the reflection probability becomes large (up to 90%) for low energy ions and neutral atoms²⁷ ($\lesssim 10$ eV), a metallic wall may be acceptable for low enough plasma edge temperatures.

B. Depolarization by diffusion

A strong source of nuclear depolarization in metals and nonmetals is close encounters between the nuclear magnetic dipole moments of diffusing D and T with nearby magnetic dipole moments, such as those of other diffusing nuclei, lattice nuclei, or unpaired bound electrons (paramagnetic

impurities). The diffusion modulates the magnetic dipole-dipole interaction

$$H_d = \sum_j \frac{\gamma \gamma_j \hbar^2}{r_j^3} \{ \hat{\mathbf{I}} \cdot \hat{\mathbf{I}}_j - 3(\hat{\mathbf{I}} \cdot \hat{\mathbf{n}})(\hat{\mathbf{I}}_j \cdot \hat{\mathbf{n}}) \}, \quad (9)$$

where $\hat{\mathbf{n}} = \hat{\mathbf{r}}_j/r_j$ is a unit vector pointing from a given diffusing nucleus at the origin to the j^{th} magnetic dipole moment. In the following, we ignore the contributions of lattice nuclei and paramagnetic moments to the sum in Eq. (9). Although this is not a good approximation - several low-Z isotopes have nuclear moments larger than that of tritium - the effects of lattice nuclei are easily included in the formalism. They can even be eliminated experimentally by using selected isotopes. The effects of paramagnetic impurities will be discussed separately below.

The depolarization rate for diffusing nuclei is given by a BPP-like formula [see Eq. (2)] where the correlation time can be shown to be $\tau_c = 1/2 \tau_D$. Here the diffusion or residence time, τ_D , is the mean time that a diffusing nucleus spends at a site before randomly hopping to a nearby (usually nearest-neighbor) available site. The depolarization rate is also proportional to c , the ratio of the number of diffusing nuclei to the number of possible lattice sites. When c is small, interactions between diffusing nuclei are rare and the depolarization rate is small.

The diffusive motion of nuclei is a thermally activated process so τ_D may be written as

$$\tau_D = \tau_0 \exp(E_{\text{act}}/k_B T), \quad (10)$$

where E_{act} is the activation energy, T is the absolute temperature, and τ_0 is a constant prefactor related to the reciprocal of the hopping attempt

frequency. E_{act} depends sensitively on the local configuration of chemical bonds.²⁹ It is small for most metals (0.1 to 0.5 eV) and large for many nonmetals (0.7 to 5 eV). The prefactor τ_0 is much less sensitive, reflecting its physical origin in lattice vibrations; it typically has a magnitude of 10^{-12} sec.

Equations (1) and (10) together predict that the longitudinal relaxation time will be smallest for temperatures near

$$T_d = - \frac{E_{act}}{k_B} \left[\ln \left(\frac{\omega_0 \tau_0}{2} \right) \right]^{-1}, \quad (11)$$

where ω_0 is the usual nuclear Larmor frequency. The prominent minimum in T_1 as a function of temperature in many experiments is then clear evidence that depolarization is dominated by diffusional motion. (Indeed, such NMR experiments provide direct information about τ_0 and E_{act} , giving insight into the microscopic diffusion pathways.¹¹) Diffusional depolarization for metals is illustrated in Fig. 2; the data are characteristic of transition metal hydrides.³⁰ There is a sharply defined minimum in T_1 near 333 K when τ_D becomes of order ω_0^{-1} . The time scale varies from ~ 20 msec near the minimum to ~ 200 msec at higher temperatures. Above 500 K, diffusion is so rapid ($\omega_0 \tau_D \ll 1$) that other depolarization mechanisms (the Korringa process, paramagnetic impurities) dominate.

Similar data are not presently available for nonmetallic wall materials such as graphite and SiC. Since the energetic flux of D and T rapidly disorders and hydrogenates the outermost layers of such materials, one might expect that nonmetallic wall depolarization rates will be similar to those of amorphous hydrogenated semiconductors (which have been widely studied in many laboratories) containing the same elements. Data on such materials show that

hydrogen and deuterium depolarization rates are an order of magnitude smaller than in metals and that the depolarization mechanisms are complex. A pronounced T_1 minimum is often found but only at temperatures too low for atomic diffusion to occur³¹ (Fig. 3). Researchers have proposed that depolarization near this minimum occurs by spin diffusion towards ortho- H_2 and para- D_2 molecules, whose magnetic moments act as (paramagnetic) relaxation centers.^{23,32} Consistent with this observation is the fact that the magnitude of T_1 is the same for many different hydrogenated (or deuterated) amorphous semiconductors.³³ Depolarization rates at higher temperatures ($T > 500$ K) have not been thoroughly studied and analyzed. Data of Carlos and Taylor^{31,34} show that the rate decreases for increasing temperature (Fig. 5), suggesting thermal diffusion with an activation energy ≈ 0.2 eV. The higher temperature rates are dependent on sample composition and history and are not understood. Further work is clearly needed.

For a given wall material, the diffusional depolarization rate can be minimized by operating at the highest possible temperature compared to T_d [Eq. (11)], assuming that T_d is not larger than the melting or sublimation temperature. For transition metal hydrides, this means $T > 500$ K (see Fig. 3). For nonmetals, the choice is less clear; it depends on the density of various traps and the distribution of trap energies. Temperatures near the sublimation point of nonmetals (~ 1400 K for graphite) may lead to unacceptable erosion rates and a large flux of wall impurities (e.g., carbon ions) into the plasma.

High operating temperatures also help reduce depolarization of deuterium nuclei by quadrupole relaxation.¹¹ The same arguments regarding the role of diffusion hold except that the dipole-dipole energy is replaced by Eqs. (4) and (5), discussed above. Provided that different sites are subject to

different electric field gradient tensors, rapid diffusive motion averages out the different environments and the depolarization rate tends to zero. The exceptions are noncubic lattice sites and diffusion near the surface, the latter often having large electric field gradients because of a redistribution of electronic charge. A calculation³⁵ shows that Raman quadrupole relaxation of deuterons on surfaces can have depolarization rates of order 0.1 sec^{-1} . If surface desorption is slow, this may be a source of depolarization.

Surface desorption processes can affect diffusive depolarization in another way. If bulk diffusivities are rapid compared to surface desorption, concentrations of interstitial D and T near saturation ($c \sim 1$) may build up below the surface. The correlation time is then no longer given by $\tau_D/2$. Instead, it depends on the mean time for a nearby site to become vacant, which can be longer than τ_D , leading to increased depolarization rates. It is not known whether such large subsurface concentrations occur in current limiters and first walls. The important rate of recombination desorption³⁶ has not been accurately measured for any surface to date. It is an important number to derive from future experiments.

C. Depolarization by paramagnetic impurities

Another source of depolarization - perhaps the major source at high temperatures for nonmetals - is unpaired bound electrons such as dangling bonds, unfilled transition (3d) or rare earth (4f) valence shells of atoms, and electrons trapped by lattice defects. Since an external field causes such electronic magnetic moments to align on the average, they are called paramagnetic impurities.

A diffusing nucleus near such an impurity can rapidly depolarize for two reasons. First, the electron magnetic dipole moment is $\sim 10^3$ times larger

than any nuclear moment; local microscopic magnetic fields are large ($\sim 10^4$ G at a separation of 10^{-8} cm). Second, unlike nuclear magnetic moments, paramagnetic impurities are strongly coupled to the lattice with spin-lattice relaxation times of order $10^{-9} - 10^{-6}$ sec. A nucleus becomes strongly coupled to the lattice in the vicinity of such an impurity and can spin-flip.

The nuclear magnetic dipole moment interacts with that of the electron by dipole-dipole and hyperfine interactions, either of which can dominate depending on chemical details.³⁷ For simplicity, we consider only the dipole-dipole contribution (the second case is discussed in detail by S.P. Vernon and collaborators).³⁸ The nuclear spin relaxation rate then depends on a balance between the rate at which nuclear spins diffuse near a paramagnetic impurity, and the rate at which the impurity can relax the nucleus by its coupling to the lattice. The latter depends on the effective magnetic moment of the tumbling electron spin, which, in turn, depends on the temperature and field-dependent electron spin-lattice relaxation time, τ_1 . Equation (1) is then no longer a sufficient criterion for the maximum depolarizing rate since a third time scale, τ_1 , enters into the physics. Although varying the temperature can decrease the nuclear depolarization rate, the dependence is not as simple as that found for diffusing nuclei interacting with other nuclei (compare Figs. 2 and 3 with Fig. 4). Because of the importance of paramagnetic impurities, we give a brief but quantitative description of how the nuclear depolarization rate depends on the various parameters.³⁹

The direct dipole-dipole interaction of a nucleus at a distance r from a paramagnetic impurity determines a relaxation time

$$\tau^{-1}(r) = Cr^{-6}, \quad (12)$$

where the interaction strength, C , is given by

$$C = \frac{2}{5} \gamma_e^2 \gamma_n^2 J(J+1) \frac{\tau_1}{1 + \omega_0^2 \tau_1^2} . \quad (13)$$

Here J , γ_e , and τ_1 are the angular momentum, gyromagnetic ratio, and longitudinal relaxation time of the impurity. τ_1 arises from spin-orbit coupling and phonon scattering and is temperature dependent, usually decreasing with increasing temperature. For $\omega_0 \tau_1 \ll 1$, the usual case, C also decreases with temperature. The quantities J , γ_e , and τ_1 can often be measured by electron spin resonance (ESR) experiments.³⁷

The paramagnetic depolarization rate, T_{1p}^{-1} , depends on the relative magnitudes of τ_D in Eq. (10) and $\tau(r)$ in Eq. (12). Alternatively, the rate depends on the relative magnitudes of two related length scales, a_1 and β . a_1 is the distance of closest approach of a nucleus to an impurity. β , the so-called pseudopotential radius, measures the effectiveness of atomic diffusion compared to direct relaxation. It is defined to be

$$\beta = (C/D_a)^{1/4} , \quad (14)$$

where D_a is the D and T lattice diffusivity. Since $D_a \sim L^2/2\tau_D$ where L is the average hopping distance, β is strongly temperature dependent by Eq. (10). The two length scales define a dimensionless parameter

$$\delta_a = \frac{\beta^2}{2a_1^2} , \quad (15)$$

which enters our discussion below.

If N is the concentration of paramagnetic impurities in cm^{-3} , and the concentration is so low that the length scale $N^{-1/3}$ is large compared to a_1 and β , the depolarization rate can be shown to be⁴⁰

$$T_{1p}^{-1} = 8\pi N D_a \beta \frac{\Gamma(3/4)}{\Gamma(1/4)} \frac{I_{3/4}(\delta_a)}{I_{-3/4}(\delta_a)}, \quad (16)$$

where β and δ_a are given by Eqs. (14) and (15), respectively. $\Gamma(x)$ is the usual gamma function and $I_{\pm 3/4}(x)$ are nonintegral modified Bessel functions. The function $I_{3/4}(x)/I_{-3/4}(x)$ is plotted in Rorschach's paper³⁹ and has a simple behavior.

Equation (16) has two interesting physical limits. When $\delta_a < 1$, diffusion is fast and relaxation is limited by the rate at which the impurity can equilibrate nuclei in its immediate neighborhood. Equation (16) then reduces to:

$$T_{1p}^{-1} \sim \frac{8\pi}{3} N D_a \beta \left(\frac{\beta^3}{2a_1^3} \right) = \frac{4\pi}{3} N C a_1^{-3}, \quad (17)$$

which is independent of D_a . An order of magnitude estimate is useful to determine what concentrations N are dangerous. For yttrium hydride with Gd^{3+} paramagnetic impurities, C can be written as $5.7 \times 10^{-38} T^{-1} \text{ sec}^{-1} \text{ cm}^{-6}$ where T is the lattice temperature.³⁰ For $a_1 \sim 1.5 \times 10^{-8} \text{ cm}$, $T \sim 600 \text{ K}$, N must be less than $\sim 10^{18} \text{ cm}^{-3}$ to make $T_{1p} \gtrsim 10 \text{ msec}$. This is roughly ten parts per million of impurity.

This fast-diffusion limit is illustrated for 90 ppm of impurity in the higher temperature region (left side) of Fig. 5. For temperatures between 350 K and 600 K, the depolarization rate is independent of temperature. This

probably reflects the increasing diffusion rate and decreasing effective electron moment, which compensate each other. For higher temperatures ($T > 600$ K), diffusion is so rapid that a single collision with the paramagnetic impurity cannot relax the nuclear moment. Figure 5 suggests that high temperatures are needed to diminish T_{1p}^{-1} . In general, the useful temperature range will depend on the particular impurity and host lattice, and is not easily predicted a priori.

The other limit occurs for $\delta_a \gtrsim 2$ and corresponds to fast impurity relaxation but slow diffusion. This is the case for large trapping energies of D and T in nonmetallic walls. Here Eq. (16) reduces to

$$T_{1p}^{-1} \sim \frac{8\pi}{3} N D_a \beta = \frac{8\pi}{3} N C D_a^{1/4} a_1^{3/4}, \quad (18)$$

and is independent of a_1 , the distance of closest approach. The rate is strongly temperature dependent, with an effective activation energy of $3/4 E_{act}$ [see Eq. (10)]. In this limit, lower temperatures are desired to decrease D_a and to reduce the depolarization rate.

The above equations assume isotropic diffusion in three dimensions. Because the wall surfaces are likely to have the highest concentrations of paramagnetic impurities, it is useful to consider the two-dimensional case. If N_s is the surface impurity concentration (in cm^{-2}), the fast-diffusion limit [Eq. (17)] becomes in two dimensions⁴¹

$$T_{1p}^{-1} = \pi N_s D_a' \left(\frac{B^2}{2} \right)^2 = \frac{\pi}{4} N_s C a_1^{-4}, \quad (19)$$

where D_a' is the surface diffusivity. Using the same order of magnitude estimate of C from yttrium dihydride,³⁰ with $a_1 \sim 1.5 \times 10^{-8}$ cm, we find that

surface concentrations $N_s \gtrsim 10^{11} \text{ cm}^{-2}$ will give $T_{1p} \lesssim 10 \text{ msec}$. This corresponds to 100 ppm on the surface. Since impurities will recycle and deposit, this is a rather likely occurrence under reactor conditions.

In the limit of slow surface diffusion, Eq. (18) becomes⁴¹

$$T_{1p}^{-1} = \frac{4\pi N_s D_a'}{\ln[(2/\pi N_s \beta^2)] - 1} \quad (20)$$

The logarithmic term in the denominator arises from diffusion in a lower dimension. This term also demonstrates that simple dimensional arguments will not suffice to determine the dependence of the depolarization rate on the relevant parameters. The temperature dependence is more complicated, but is still dominated by D_a' in the numerator.

All the above formulas are valid in the limit of dilute impurity concentrations, when diffusing nuclei interact on the average with only one impurity. The surface is likely to violate this restriction by having large concentrations. The surface may therefore be a major source of nuclear depolarization if most impurities can relax the nuclei. Little is known about this possibility. Some kinds of paramagnetic impurities such as trapped electrons or dangling bonds will bind hydrogen and become neutralized. Other paramagnetic impurities with unfilled d or f valence shells cannot be eliminated by binding with surface hydrogen. However, their effective magnetic moments may be small if surface spin-relaxation is rapid; electron spin resonance measurements of highly dispersed powders may illuminate this case. Finally, at high impurity concentrations, nuclei interact with several impurities at once and impurities interact with each other, a complex situation which is not understood even in principle.⁴² We urge further theoretical and experimental work to investigate the importance of surface

paramagnetic impurities.

5. CONCLUSIONS

The earlier sections have explained in detail some of the physical principles which govern the rate of depolarization of D and T nuclei which recycle many times at material walls. Our discussion is summarized in Tables 2 and 3 which list, respectively, the qualities we think a first wall or limiter should have and some possible wall materials. This summary should be considered indicative rather than definitive in view of the complexity and diversity of possible depolarization mechanisms in crystal lattices.

Our discussion suggests that depolarization of the plasma by recycling in material walls is far more important than depolarization in the plasma core. Instead of depolarization rates $\lesssim 10^{-5} \text{ sec}^{-1}$ in the core, we can expect rates $\lesssim 1 \text{ sec}^{-1}$ for nonmetallic walls at high temperatures. For some parameters, the mean residence time can be less than the longitudinal relaxation time.¹² This gives us cautious optimism that suitable wall and limiter materials can be found. Clearly, however, systematic experimentation will be required to improve our understanding.

The experimental data presented in Sec. IV suggest that hydrogenated (or deuterated) amorphous semiconductors might be an interesting candidate material. Several other reasons strengthen this proposal. First, a coating over the limiter and walls would be easy to apply by introducing puffs of methane or silane during low-current discharges; the reactor need not be turned off and opened to apply new coatings. Second, because these materials have high concentrations of D and T already present, the flux of lattice nuclei into the plasma (a source of higher Z impurities) might be decreased compared to crystalline graphite or SiC. Third, small amounts of dopants such

as nitrogen could be used to tune the longitudinal relaxation time, and perhaps the residence time. Finally, the porosity of the coating could be varied by controlling the deposition rate. This can reduce the depolarization rate by providing a loose network of channels through which polarized nuclei can escape back to the surface. Many of these conjectures can be tested directly by NMR studies of plasma-deposited hydrogenated amorphous semiconductors at higher temperatures than those studied to date.

There are several depolarization mechanisms whose magnitudes are unknown. Most important is the possible role of large concentrations of surface paramagnetic impurities. Such impurities can be systematically studied in two ways. One is to use NMR to study highly dispersed particles²⁶ coated with hydrogen and with possible wall impurities such as Ti, Fe, Mo, Gd, etc. The second approach is to scatter low energy polarized alkali nuclei⁴³ off carefully prepared surfaces in an ultra high vacuum chamber. Measurement of the depolarization rate of desorbed nuclei would then give information about the relaxation times of nuclear spins on the surface. This technique is still in its infancy and has not yet become a quantitative tool. It is quite promising though, since it can also give information about surface hydrogen diffusivities and concentrations, data that are sorely lacking when one wants to calculate the bulk concentration profile governing the wall residence time.

Other experiments were mentioned in the previous sections. They include studying the importance of spin-rotation relaxation in voids and cracks, the measurement by NMR of bulk diffusivities in nonmetals, ESR measurements of paramagnetic electron relaxation times, and the role of lattice nuclear magnetic moments and bulk paramagnetic impurities. Since depolarization rates are so slow in the plasma core, the decrease in enhancement of D-T reactions of polarized nuclei could be a direct measure of the total depolarization rate

arising from plasma edge, surface, and bulk processes. This would make an interesting experiment for testing future limiter and wall candidates.

In conclusion, our review and discussion of NMR theory and experiment give us reasonable hope that suitable wall and limiter materials can be found. We suggest that hydrogenated amorphous semiconductors are a promising class of materials - easily applied as a coating - which merits further investigation. Experiments are suggested to measure the importance of depolarization mechanisms whose magnitudes are currently unknown. Finally, we emphasize that the proposed NMR experiments are directly useful in giving us information about the wall under reactor conditions, information that is also needed for the success of the magnetic confinement fusion effort.

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TABLE 1. Parameters for H, D, T, and e

Spin	Gyromagnetic Ratio γ rad sec ⁻¹ G ⁻¹	Magnetic dipole moment units of μ_N (5.05×10^{-24} ergs G ⁻¹)	Electric quadrupole moment, Q, in cm ²
H 1/2	2.68×10^4	2.79	0
D 1	0.411×10^4	0.857	2.77×10^{-27}
T 1/2	2.85×10^4	2.98	0
e 1/2	1.76×10^7	1836	0

TABLE 2. Desirable Properties of Wall and Limiter Materials

PROPERTY	COMMENTS
High temperature	reduces dipole, quadrupole, and paramagnetic relaxation; decreases residence time.
Nonmetallic materials	eliminates relaxation due to inelastic spin-flip collisions with conduction electrons.
Lattice nuclei have small or zero magnetic dipole moments	decrease diffusional relaxation.
High H and He solubilities	avoid blistering of wall which can lead to internal sources of diatomic molecules and spin-rotation relaxation.
Rapid surface desorption by molecular recombination	minimize residence time by allowing nuclei to escape rapidly.
Low-Z atomic composition	avoid high-Z impurities in plasma that lead to high radiation loss.
Low surface and bulk concentrations of paramagnetic impurities	not easily controlled because of constant erosion and redeposition.
Cubic lattice symmetry	noncubic lattice sites can depolarize deuterons by quadrupole relaxation.

TABLE 3. Candidate Wall Materials

MATERIAL	COMMENTS
Hydrogenated amorphous semiconductors (a - Si:H) (a - C:H)	best choice based on current knowledge
Graphite	long residence times might off- set slow depolarization rates
SiC	see graphite comments

FIGURE CAPTIONS

FIG. 1. Schematic illustration of the plasma-wall interaction. The partially ionized cooler plasma near the wall is the plasma edge; diatomic and triatomic molecules in this region are the major source of edge depolarization. About 50% of incident ions (dark circles) are reflected by lattice atoms (open circles). Remaining nuclei enter the lattice and diffuse or become trapped. Nuclei on the surface desorb either by recombination or by collisions with incoming photons, electrons, and ions.

FIG. 2. Longitudinal relaxation time (T_1) versus reciprocal temperature for typical transition-metal hydrides (based on Ref. 30). The pronounced minimum at 333 K is indicative of diffusional depolarization (dash-dot line, labeled T_{1d}). At higher temperatures, Korringa or electronic relaxation (dashed line, labeled T_{1e}) by conduction electrons dominates. At lower temperatures, relaxation by paramagnetic impurities (solid line, labeled T_{1p}) dominates if they are present. The higher temperature part of T_{1p} is now known to have a different behavior (see Fig. 5 and Ref. 30).

FIG. 3. Longitudinal relaxation time (T_1) versus temperature for hydrogenated and deuterated amorphous silicon (see Refs. 31 and 32). The closed and open circles and squares are data from different samples prepared by a glow-discharge method; the triangles are data taken on samples which were prepared with little or no H_2 present. The pronounced minimum in T_1 near 30 K is due to spin diffusion towards paramagnetic centers ($H_2^{\cdot}$). Away from this minimum, T_1 is an order of magnitude larger (> 2 sec) than the values for metals (Fig. 2). We are indebted to Dr. R. Norberg for this data.

FIG. 4. Longitudinal relaxation rate (T_1^{-1}) versus reciprocal temperature for hydrogenated amorphous silicon (Ref. 34). At higher temperatures, the depolarization rate increases. The physical mechanism is not well understood and needs to be further investigated.

FIG. 5. Longitudinal relaxation rate (T_{1p}^{-1}) of hydrogen nuclei versus reciprocal temperature for paramagnetic impurities (100ppm Gd) in $\text{LaH}_{2.26}$ (based on Ref. 30). For $T \gtrsim 300$ K, T_{1p}^{-1} is roughly constant over a range of two hundred degrees. For $T \gtrsim 600$ K, the fast diffusion regime is entered and the depolarization rate decreases. Different behavior will be found for different impurities and lattices, although the qualitative behavior will be similar.

83P0222

Fig. 1

Fig. 2

#84P0021

Fig. 3

83P0248

Fig. 4

#84P0022

Fig. 5

EXTERNAL DISTRIBUTION IN ADDITION TO TIC UC-20

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