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Retention Count Based Material Reliability Calculation for Molecular Dynamics of Tritium Plasma at Graphene

Grafende Tritiyum Plazmasının Moleküler Dinamikleri için Tutma Sayısına Dayalı Malzeme Güvenilirliği Hesaplaması

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Makale Bilgisi

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Highlights

It was investigated the effect of tritium plasma ions with energy ranging from 5 to 35 keV on graphene walls using molecular dynamics simulations. Based on these energies, retention counts of the graphene is used to calculate the Weibull reliability which showed the reliability of the structural material.

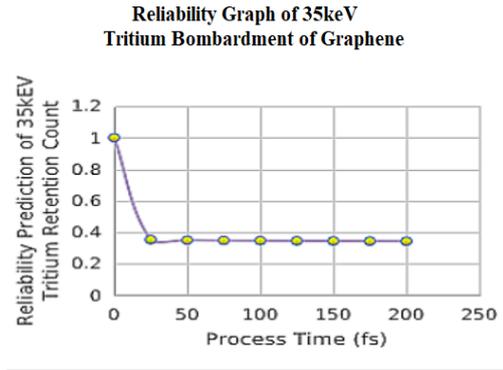
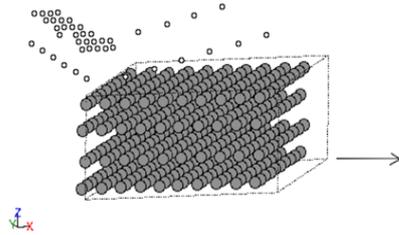
Keywords

PMI retention count
Material reliability
retention count
Weibull Reliability
based with retention
count

Graphical Abstract

Anahtar Kelimeler

PMI tutma sayısı
Malzeme güvenilirliği
tutma sayısı
Tutma sayısına
dayalı Weibull
Güvenilirliği



Abstract

Structural dependability of Tokamak fusion reactors has to be taken into account while selecting reactor components. Heat- and energy-producing fusion events can change reactor walls. Reactions thus produce less efficiently the energy needed. For example, graphene is the fundamental building block used in fusion reactors to create their walls. Among the newest high-tech materials is graphene. In the study, it was investigated the effect of tritium plasma ions with energy ranging from 5 to 35 keV on graphene walls using molecular dynamics simulations. Based on these energies, retention counts of the graphene is used to calculate the Weibull reliability which showed the reliability of the structural material. To study the surface topology, we calculate the tritium retention count, since molecular dynamics gives a snapshot of the actual world in the molecular model setup. The surface tritium plasma atom retention calculation is completed by determining the graphene's Weibull distribution reliability based on the retention count assumption.

Özet

Tokamak füzyon reaktörlerinin yapısal güvenilirliği, reaktör bileşenleri seçilirken dikkate alınmalıdır. Isı ve enerji üreten füzyon olayları reaktör duvarlarını değiştirebilir. Bu nedenle reaksiyonlar ihtiyaç duyulan enerjiyi daha az verimli üretir. Örneğin, grafen, füzyon reaktörlerinin duvarlarını oluşturmak için kullanılan temel yapı taşıdır. En yeni yüksek teknoloji malzemeler arasında grafen de yer almaktadır. Moleküler dinamik simülasyonları kullanarak, 5 ila 35 keV arasında değişen enerjiye sahip trityum plazma iyonlarının grafen duvarları üzerindeki etkisini araştırmış olup, bu enerjilere dayanarak, grafenin tutulma sayıları, yapısal malzemenin güvenilirliğini gösteren Weibull güvenilirliğini hesaplamak için kullanılmıştır. Yüzey topolojisini incelemek için, moleküler dinamikler moleküler model kurulumundaki gerçek dünyanın bir anlık görüntüsünü verdiği için, trityum tutma sayısı hesaplanmıştır. Yüzey trityum plazma atom tutma hesabı, tutma sayısı varsayımına dayalı olarak grafenin Weibull dağılımının güvenilirliğini belirleyerek tamamlanmıştır.

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1. INTRODUCTION

A significant challenge this century is the increasing demand for energy, which is a result of the increasing population and living standards. Most energy comes from depleting fossils. Sustainability requires nuclear and renewable energy [1-2]. End-exothermic nuclear reactions provide energy. Nuclear reactions like fission and fusion are vital. Energy arises from a massive, unstable nucleus shattering. Fission powers most nuclear reactors. Nuclear fusion fuses several nuclei. It makes nukes and subatomic particles. Mass changes in reactants and products provide energy. Fusion requires 100 million degrees. Nuclear fusion gives practically unlimited fuel worldwide. Fusion reactors produce transient radioactive waste using safety mechanisms [3-6]. The most famous fusion reaction uses tritium and deuterium. The 14.1 MeV neutron from this event warms water to make turbine steam. Additionally, this reaction yields 3.5 MeV He [7-10]. Helium reactors heat plasma [11-15]. Classic thermonuclear fusion reactors use magnetic fields to densify plasma. Figure 1 shows magnetic fields trap plasma from the reactor's first wall. Plasma strength affects barriers. The divertor zone has the highest attrition because magnetic field lines convey lower-energy plasma to the wall. Explore plasma-first wall interactions and materials.



Figure 1: A nuclear fusion reactor (Tokamak).

Plasma fuses helium. Helium reacts with divertor walls after removal [16–18]. Failure of the fuel diverter and reactor walls releases neutrons. Tokamak reactor walls are protected with tungsten, beryllium, molybdenum, steel, and graphene. High melting point and atomic number make tungsten plasma-resistant [16–19]. Few studies have addressed fission reactor structural reliability. Reference [19] examines nuclear fission reactor structure, length, reliability, and risks associated probabilities, material science effects, reactor pipeline fluid effects on structure and their corrosion created fractures, and structural mechanics deformation mechanisms. Many nuclear fusion devices have fusion reaction issues. Literary sources don't emphasize organizational trust. There has been a recent surge in structural and thermomechanical research [20]. Discussing diagnostic, magnet, and reproduction covers. Safe and reliable systems affect fusion device reliability. Teaching faith. The availability, maintainability, and inspectability of Wendelstein 7-X, DEMO, and ITER fusion equipment for experiments or energy generation are reviewed [21]. This study covers solely fusion device basics. Commercial plasma with surface coating is best for testing the reliability of Tokamak fusion reactor structures. Plasma-exposed spacecraft must resist radiation and particles. To avoid space effects, plasma-facing buildings must regulate radiation and particles [22–24]. Tritium proved challenging to retain in tokamak walls. Plasma-facing graphene magnetic fusion loses tritium. 40% of plasma tritium was preserved by JET, 51% by TFTR. After tests, 12–16% of the fusion reactor needed

cleaning. Titanium walls are strong. New computer estimates reveal that the French experimental Tokamak reactor ITER will run out of tritium after 100 bursts. Tritium degrades reactor walls. This impacts fusion heat-to-electricity. This study created a graphene wall with larger crystalline atomic patterns using molecular dynamics models. Figure 2 shows the simulation's first research model.

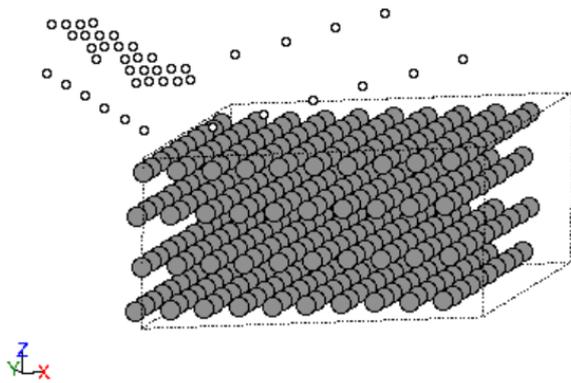


Figure 2: Atomic simulation system startup model configuration for Tritium and Graphene surface crystal.

2. METHOD

Many nuclear fusion devices have fusion reaction issues. Literary sou The retention mechanism for a substantial quantity of graphite, which contains nearly 1,200 carbon atoms, was modeled in this study. The results indicated that the retention efficiency was susceptible to a variety of parameters, including the simulated pressure and temperature. These results have the potential to significantly influence future research on carbon-based materials and their applications in various industries. In order to facilitate calculations with the 3T magnetic induction force application, we subjected the block to hydrogen at energy levels ranging from 5 to 35 keV, which replaced tritium. These energies are selected based on the literature

of the plasma molecular dynamic studies that use ion ranges in the 1-100 keV energy range [28]. The fact that the simulation functioned satisfactorily at these energies implies that the existing models encompass a respectable range of collision energies as reported in the literature. The objective of this research was to create a model that could generate tritium retention counts on the surface in order to determine reliability. The interaction between tritium plasma atoms and graphite could be investigated by constructing this model using molecular dynamics simulations. Python is employed by to the study to conduct molecular dynamics simulations. For this purpose, we employ Spyder (Scientific Python Editor) 6.0.3, a component of the Anaconda package. The calculations are executed on a Dell Precision 7680 using Ubuntu 24.10 Linux and an Intel Core i7 13th Gen processor. The Python compiler version 3.12.7 was implemented. The Atomic Simulation Environment (ASE), a molecular dynamics simulation program that is Python-based, is employed in this research [25]. After the molecular dynamic simulation is executed, retention count for the Tritium atoms are calculated in the graphene surface which the pseudo code is given below applied:

1-Initialize lists for atom indices:

- a) *Create empty lists of H atoms*
- b) *Create empty lists of C atoms*

2-Identify H and C atoms:

- a) *Loop through the H or C list (from index 0 to length-1:*
 - i. *if the symbol at the current index H, append the index to H indices*

- ii. if the symbol at the current is C, append the index to C indices

3-Initialize retention counter:

- a) Set retention count to 0 to keep track of qualifying H atoms.

4-Check H atom for nearby C atoms:

- a) For each H index in the H indices list:
 - i. Retrieve the 3D position of H atom
 - ii. Set flag to track if a nearby C is found.

- iii. For each C index in C indices:

1. Retrieve the 3D position of the C atom
2. Calculate the Euclidean distance between H position and C position
3. If distance < 2 Angstrom (cut of distance) increment retention count by one, set C found to True and break out of the inner C loop

5-Return result:

- a) After all H are processed, return retention count (the number of H atoms near at least one C atom within the cut of distance)

The reliability distribution of the Weibull probability is computed based on the calculated retention count values. The equation for the three-parameter Weibull distribution is presented as follows [27]:

$$R(t) = e^{-\left(\frac{t-\gamma}{\alpha}\right)^\beta} \quad (1)$$

in which t represents the duration of irradiation, γ denotes the location parameter, β denotes the shape parameter (slope) with $\beta > 0$, and α denotes the scale parameter (characteristic life) with $\alpha > 0$.

In calculations, it is commonly understood that $\gamma=0$, as it denotes the displacement of the origin of the reliability distribution graph. The failure probability function is specified as follows:

$$F(t) = 1 - R(t) \quad (2)$$

$$1 - F(t) = e^{-\left(\frac{t}{\alpha}\right)^\beta} \quad (3)$$

In the previously mentioned context, $\gamma=0$, and based on the established criteria for F(t), it is true that 0:

$$\ln\left(\ln\frac{1}{1-F(t)}\right) = \beta \ln t - \beta \ln \alpha \quad (4)$$

The following expression is generated in order to formulate the equation in the configuration of $y=mx+n$:

$$y(t) = \ln\left(\ln\frac{1}{1-F(t)}\right), m = \beta \text{ and } n = -\beta \ln \alpha \quad (5)$$

The Bernard Approximation for Median Ranks is employed to compute the unreliability parameters for each failure [29]. In the above (5) Weibull calculation α and β is calculated by the application of the linear trendline on a graph represents the result of linear regression based on the y(t) plotted points. Subsequently, we determine the unreliability parameter.

$$F(t) = \text{MedianRank} = \frac{\text{Rank} - 0.3}{N + 0.4} \quad (6)$$

Let N represent the maximum number of trials with different input energy levels between 5keV to 35keV under 3T magnetic induction force in the molecular dynamics dataset, and let rank denote the order number as presented in the tables within the results section.

3. RESULTS AND DISCUSSION

In order to bombard the graphene crystal with hydrogen ions, the simulation employs a magnetic field strength of 3T, with energy levels ranging from 5 keV to 35 keV. The next stage of the procedure entails conducting molecular dynamics simulations. The multilayered construction of graphene facilitates the integration of thermostats. This sequence outlines the calculations of retention counts for atoms within molecular configurations and presents the results of the three-dimensional molecular dynamics simulation. Tables 1, 2, 3, and 4 present the retention count derived from the molecular simulation model. These tables include the corresponding rank, the F(t) function, the natural logarithm of the retention count, the y(t) function associated with the retention count, and the reliability calculated from the y(t) function for tritium exposed to kinetic energies ranging from 5 keV to 35 keV under a 3T magnetic induction force.

Table 1: Retention Count for F(t) and y(t) values calculated by equations 2, 3, 4, 5 and 6 for Tritium with 5keV.

Process Time Step (fs)	Retention Count of the Tritium on the surface	Rank	F(t)	ln(Retention)	y(t)_Retention
0	9	1	0,074	2,197	0
25	11	2	0,181	2,397	0,3770
50	7	3	0,287	1,945	0,3790
75	9	4	0,394	2,197	0,380
100	11	5	0,5	2,397	0,381
125	10	6	0,606	2,302	0,381
150	9	7	0,712	2,1972	0,382
175	9	8	0,819	2,1972	0,383
200	8	9	0,925	2,0794	0,383

Table 2: Retention Count for F(t) and y(t) values calculated by equations 2, 3, 4, 5 and 6 for Tritium with 15keV.

Process Time Step (fs)	Retention Count of the Tritium on the surface	Rank	F(t)	ln(Retention)	y(t)_Retention
0	9	1	0,074	2,197	1
25	9	2	0,180	2,197	0,290
50	12	3	0,287	2,484	0,275
75	12	4	0,394	2,484	0,266
100	12	5	0,5	2,484	0,259
125	12	6	0,606	2,485	0,2545
150	13	7	0,713	2,565	0,251
175	14	8	0,819	2,639	0,247
200	16	9	0,925	2,772	0,244

Table 3: Retention Count for F(t) and y(t) values calculated by equations 2, 4, 5 and 6 for Tritium with 25keV.

Process Time Step (fs)	Retention Count of the Tritium on the surface	Rank	F(t)	ln(Retention)	y(t)_Retention
0	9	1	0,074	2,197	1
25	9	2	0,180	2,1972 24577	0,290
50	12	3	0,287	2,485	0,274
75	12	4	0,393	2,485	0,265
100	12	5	0,5	2,485	0,259
125	12	6	0,606	2,485	0,254
150	13	7	0,713	2,565	0,250
175	14	8	0,819	2,639	0,247
200	16	9	0,925	2,772	0,244

Table 4: Retention Count for F(t) and y(t) values calculated by equations 2, 4, 5 and 6 for Tritium with 35keV.

Process Time Step (fs)	Retention Count of the Tritium on the surface	Rank	F(t)	ln(Retention)	y(t)_Retention
0	9	1	0,074	2,197	1
25	10	2	0,180	2,302	0,352
50	12	3	0,287	2,484	0,349
75	13	4	0,393	2,565	0,347
100	11	5	0,5	2,398	0,346
125	12	6	0,606	2,485	0,345
150	9	7	0,713	2,197	0,343
175	11	8	0,819	2,398	0,343
200	12	9	0,925	2,485	0,342

Many nuclear fusion devices have fusion reaction issues. In the above tables ln(retention count) column is used to calculate the values of y(t)_retention columns based on the trendline functions slope equations given in (6). Then the last column is computed with the equation (3) to calculate the reliability of the materials based on the retention and the resultant graphs are given in the figures 3, 4, 5, 6:

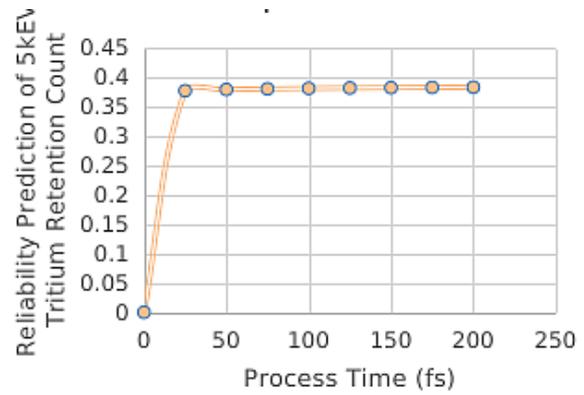


Figure 3: Tritium and Graphene surface crystal Calculated reliability of retention count of the simulated system based on 5keV bombardment of Tritium.

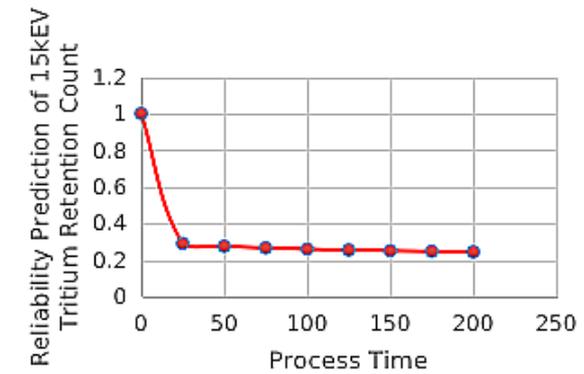


Figure 4: Tritium and Graphene surface crystal Calculated reliability of retention count of the simulated system based on 15keV bombardment of Tritium.

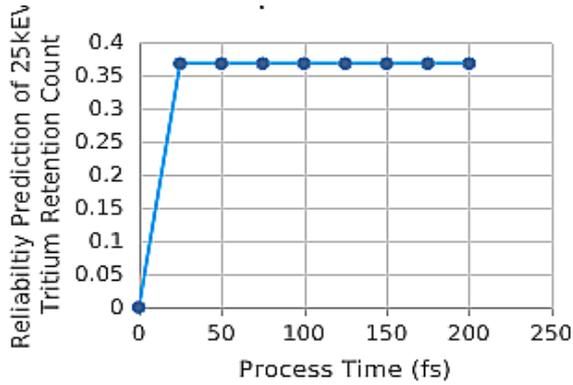


Figure 5: Tritium and Graphene surface crystal Calculated reliability of retention count of the simulated system based on 25keV bombardment of Tritium.

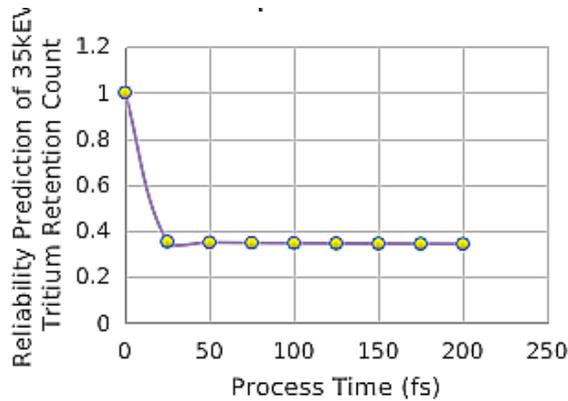


Figure 6: Tritium and Graphene surface crystal Calculated reliability of retention count of the simulated system based on 35keV bombardment of Tritium.

Subsequently, Figures 3, 4, 5, and 6 are analyzed. The two graphs given in figure 4 and figure 6 demonstrate a resemblance to the probability density function of the Weibull distribution's hazard function. Since the figure 4 and figure 6 is based on the 15keV and 35 keV bombardment tritium plasma ion process, the retention of the tritium ions showed the similar retention count distribution pattern on the graphene structure. The assessment of the graphene crystal material's reliability will be conducted

through the retention count, a metric indicating the quantity of material accumulated within the crystal structure.

4. CONCLUSIONS

The evaluation of material selections necessary for plasma-based energy devices, including fusion Tokamak reactors and space propulsion systems, is facilitated by the graphs presented in the previous results. Structures' reliability in their interactions with plasma and materials is assessed by the Weibull distribution, which employs calculations derived from retention count, as demonstrated by the estimated results. This method is currently employed by the nuclear fission sector to predict structural reliability. The reliability of the material will be examined in future experiments by examining the impact of plasma collisions and the ability of graphene surfaces to retain tritium. This analysis illustrates that the tritium used in the plasma core to maintain its position will influence the design of Tokamak fusion reactors that employ graphene surface panels. The simulation results indicate that the interactions between carbon and hydrogen atoms may result in a larger quantity of tritium being retained by graphene layers. Some of them (Figure 6-8 Reliability Graphs) are creating chemical bond and some of them directly accumulated on the surface. Studies on molybdenum, beryllium, and tungsten are currently being conducted in the literature. It is also

recognized that boron-rich materials, including glass systems based on boron oxide, or richer compounds like graphene or other fusion reactor wall structures may offer resistance to plasma effects. For this, further research on molecular dynamic modeling for glass systems based on boron oxide will be looked at. This analysis suggests that the wall structures of Tokamak fusion reactors, including the International Thermonuclear Experimental Reactor (ITER) of the European Union, will incorporate a variety of materials, including tungsten, rather than graphene.

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AUTHOR CONTRIBUTIONS

Alper PAHSA: Conceptual Design, Literature review, Methodology, Analysis evaluation, Data Analytics

CONFLICTS OF INTEREST

During the investigation, no conflicts of interest, whether financial or otherwise, were identified. The study failed to comply with the ethical standards established by recognized publication and research guidelines, as it did not secure informed consent from either human participants or animal subjects.

DATA AVAILABILITY

The conclusions of the study are substantiated by the text and supplementary resources. Supplementary data pertinent to the investigation may be furnished by the corresponding author upon reasonable request.

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