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Quantum Homodyne Analysis of Molecular Dynamics Simulation of TiB_2 Crystal with Deuterium Plasma Interaction †

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Abstract

Plasma–material interactions and structural studies are needed for tokamaks. High-energy plasmas alter surfaces. Surface modification requires chemical or physical sputtering and retention. This study evaluates the molecular dynamics simulation model of TiB_2 interacting with deuterium plasma during sputtering using quantum homodyne analysis. Homodyne probabilities from deuterium-ion sputtering deformed TiB_2 in simulations. TiB2 and deuterium ions interacted at particular temperatures, magnetic fields, and kinetic energies. This study will improve first-wall fusion reactor materials. TiB_2's deuterium plasma stability and durability need further study. This may help us imagine its uses. Quantum computing using plasma–material interactions analyzes quantum homodyne.

Keywords: PMI; quantum computing in nuclear; PMI homodyne analysis

1. Introduction

Fusion reactors are the best option for creating energy (Figure 1). This application is optimal because of its limitless fuel source and the absence of radioactivity. From hydrogen-based fuels, nuclear fusion reactions within the core plasma of fusion energy reactors generate energetic particles, including neutrons and helium [1–5]. Nuclear fusion is the process of combining two nuclei to form a single, larger nucleus. The fusion of two positively charged particles is impeded by Coulomb repulsion, which also inhibits the attraction of their nuclear forces. The nuclear force is short-range and extends only barely beyond the nuclear "surface." The energy barrier is generated by the repulsive Coulomb force, which is long-range. The Coulomb barrier is contingent upon the charges and radii of the two interacting nuclei. Two protons are separated by the 400 keV energy barrier. The barrier is significantly augmented by charged particles. This configuration is frequently implemented in plasma environments. Plasma ions and electrons travel independently as a result of external electrical neutrality. Ions and electrons must traverse a helical path around the field lines in fusion reactors that are equipped with a magnetic field. Magnetic confinement is implemented in Tokamak fusion reactors [6–9].

Classical molecular dynamics (MD) is a useful tool to simulate plasma–material interactions (PMI); yet, it suffers from the inherent limits of post-process analysis and classical MD itself. In particular, they fail to capture the macro-scale uncertainties associated with stochastic ion bombardment, the loss of quantum coherence in lattice vibrations during high-energy cascades, or a unified mathematical description of continuous observables such as atomic displacements and momentum transfers. In this work, we provide a continuous-variable (CV) quantum approach to fill these gaps. Within this paradigm, the local lattice displacements

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(Δx), the change in momentum (Δp), and the field-driven perturbations during sputtering are directly mapped onto the quadrature operators $\hat{x}$ and $\hat{p}$. This mapping establishes a link between atomistic kinematics and a quantum phase-space representation, where every ion impact event can be viewed as a measurement-triggered collapse of a continuous quantum state. Thus, the quantum homodyne method is applied not only as a new method but also as a mathematical diagnostic tool that can describe the continuous changes in phase space of the destroyed TiB_2 lattice under deuterium plasma exposure.



Figure 1. DIII-D National Fusion Facility in San Diego.

Selecting a plasma-facing material is one of the most significant obstacles to commercial fusion energy. PMI erosion on ultra-high-temperature ceramic (UHTC) TiB_2 was studied utilizing deuterium and helium plasma. This study used literature-researched, reaction hot-pressed TiB_2. PFM applications benefit from TiB_2's thermal transport and high-temperature strength. Mid-Z diborides are intended for main-wall sacrificial limiters, where energetic charge-exchange neutral fluxes are high and sputtered materials migrate into the core plasma more than divertor materials. Limiter PFMs focus on lower-Z materials and plasma compatibility to decrease radiative cooling and restrict the effect of sputtered materials on reaction efficiency because core plasma tolerance for heavy refractory metals like tungsten is limited.

A variety of factors affect plasma–material interactions. Chemical activities occur at such rapid rates (picoseconds to nanoseconds) that post-process analysis of the wall material cannot determine the degree of alteration. The atomic length scales involved complicate the understanding and quantification of the intricate reaction dynamics of surface evolution, ion implantation, and bombardment. Typically, high-fidelity quantum mechanical simulations cannot address these issues. Molecular dynamics (MD) and other atomistic modeling approaches have gained significance in the characterization of PMIs. Furthermore, the quantum dimension of MD analysis, as applied in homodyne measurement, is an innovative technique that has been recently introduced in this field. This analysis elucidates the multidimensional input and output associated with the molecular dynamics of TiB_2 sputtering under deuterium-ion plasma, conducted using Python 3.13.9 within a specialized atomic modeling environment, plasma processing, and a Deep Quantum library, as documented in the open-source literature.

2. Materials and Methods

Atom modeling and molecular dynamics (MD) have gained significance in elucidating the nature and functionality of PMIs. This study primarily focuses on the molecular physics underlying the tritium retention process on the walls of a deuterium reactor. In continuous-variable (CV) quantum computing, homodyne detection is a crucial and very effective measurement technique. Various forms of quantum light states, such as vacuum, squeezed, and coherent states, can be characterized by examining the quadratures of the

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electromagnetic field (amplitude or phase). The interaction between TiB_2 and deuterium ions was modeled utilizing the kinetic energy of the deuterium ions, the temperature of the system, and an applied magnetic field. A homodyne analysis was conducted via quantum computing. Python served as the programming language for all calculations and research activities. An atomic modeling environment package from the open-source literature was utilized, in conjunction with the Python programming language. A substantial quantity of TiB_2 crystal, comprising around 1610 atoms and 10 deuterium atoms deposited on its surface, was sputtered in a manner analogous to real-world conditions for the investigation. The deuterium-ion energy range (40–2000 keV) was taken directly from the reference literature on plasma research and served as a baseline for accelerated stress testing. The approach, although above typical Tokamak edge/divertor regimes (eV to a few keV), enabled us to see sputtering and lattice degradation during realistic simulation times without changing the fundamental collision physics.

Traditional MD data from ASE (positions and velocities) were coarse-grained into mean quadrature values ($\hat{x}$) and (p_x), and then they were traced to quantum operators $\hat{x}$ and $\hat{p}$ given in Table 1. For each trial, the Deep Quantum library started with a displaced squeezed vacuum state for (1):

$$\rho = \hat{D}(\alpha)\hat{S}(\varepsilon)|0\rangle\langle 0|\widehat{S^{\dagger}}(\xi)\widehat{D^{\dagger}}(\propto), \quad (1)$$

Homodyne detection interferes ρ with a local oscillator, sampling $P(x_\theta) = \langle x_\theta|\rho|x_\theta\rangle$. The measurement deformed the state, resulting in continuous outputs aggregated across 250 trials to generate homodyne plots and Table 2. Deuterium plasma ions impacted the block, while the energy level ranged from 40 keV to 2000 keV. The energies were sufficient to conduct the simulation, indicating that the existing models encompassed a broad spectrum of collision energies. We developed a molecular dynamics computer model [2] to investigate the interaction between TiB_2 and deuterium as a plasma ion and its impact on the material's structure and chemical processes. Classical molecular dynamics (MD) is a computational method that employs the summation of Newton's second law of motion to simulate the movement of a collection of particles (atoms or molecules).

Table 1. Quantum parameters for this study.

Phase (θ)	Measured Quadrature	Physical Analogy
0	$\hat{x}$	"Position"
$\pi/2$	$\hat{p}$	"Momentum"
Arbitrary	$\widehat{x_\theta}$	Rotated phase-space coordinate

Table 2. Quantum circuit analysis of the TiB_2 crystal under deuterium plasma-ion process.

No.	Initial Beam Energy (keV)	Initial System Temperature (K)	Position Uncertainty (X, Y, Z)	Mean Position (X, Y, Z)	Entanglement Entropy	Mean Coherence Length
1	40 keV	513.15 K	(4, 2.16, 0.33)	(8.9, 8.7, 36.9)	1.0986	9.1261 Å
2	40 keV	1073.15 K	(4.9, 2.8, 0.48)	(9.44, 3.2, 37)	1.3863	9.2784 Å
3	90 keV	513.15 K	(7.5, 7.04, 1.16)	(6.38, 17.3, 37.4)	1.0986	20.7734 Å
4	90 keV	1073.15 K	(1.09, 11.4, 1.07)	(2.96, 16.2, 38.1)	1.0986	23.0329 Å
5	150 keV	1200 K	(0, 0, 0)	(19.6, 18.9, 36.3)	0.6931	0 Å

A basic method used in continuous-variable (CV) quantum computing to find the quadrature operators of a quantum state is homodyne measurement. In contrast with discrete-qubit systems that assess |0> rangle or |1>, CV systems evaluate continuous attributes such as position or momentum. In a CV system, it is formulated as the bosonic

creation ($a^{\dagger}$) and annihilation (α) operators. From these, Hermitian quadrature operators are derived, which are analogous to position ($\hat{x}$) and momentum ($\hat{p}$) for (1):

$$\widehat{x} = \frac{1}{\sqrt{2}}(\alpha + a^{\dagger}), \tag{2}$$

$$\widehat{p} = \frac{i}{\sqrt{2}}(a^{\dagger} + \alpha), \tag{3}$$

A general quadrature operator at a phase angle is defined as

$$\hat{x}_0 = \hat{x}\cos\theta + \hat{p}\sin\theta, \tag{4}$$

The goal of homodyne detection is to measure $\hat{x}_0$ by interfering with the signal state using a high-intensity reference beam called the local oscillator (LO). The signal state $\hat{a}_S$ and the local oscillator $\hat{a}_{LO}$ are combined in a 50:50 beam splitter. The LO is a classical-like coherent state with a large amplitude $\alpha = |\alpha|e^{i\theta}$. The output modes of the beam splitter are $\widehat{c_1} = \frac{1}{\sqrt{2}}(\hat{a}_{LO} + \hat{a}_S)$ and $\widehat{c_2} = \frac{1}{\sqrt{2}}(\hat{a}_{LO} - \hat{a}_S)$. Two photo-detectors measure the intensity (photon number) of the output modes. The difference in the resulting photo-currents ($\Delta\hat{n}$) is calculated as follows:

$$\Delta\hat{n} = \hat{c}_1^{\dagger}\hat{c}_1 - \hat{c}_2^{\dagger}\hat{c}_2 = \widehat{a_{LO}^{\dagger}}\hat{a}_S + \hat{a}_S^{\dagger}\hat{a}_{LO}, \tag{5}$$

Because the local oscillator is very intense, it can be configured as a classical complex number α. Substituting into the difference equation results in

$$\Delta\hat{n} \approx |\alpha|(\hat{a}_S e^{i\theta} - \hat{c}_2^{\dagger}\hat{c}_2 = \hat{a}_S^{\dagger}e^{i\theta}) = \sqrt{2}|\alpha|\widehat{x_\theta}, \tag{6}$$

By scaling the current by $\frac{1}{\sqrt{2|\alpha|}}$, a direct measurement of the quadrature $\widehat{x_\theta}$ is obtained.

In the open-source Deep Quantum [7] library or similar CV frameworks, homodyne measurement collapses the quantum state into an eigenstate of the operator $\widehat{x_\theta}$. The result is a continuous real number, which is a minimum requirement for Gaussian quantum calculations and protocols like quantum teleportation. Based on this theory, the Deep Quantum Python platform was used to perform a homodyne calculation of the MD simulation of TiB_2 under deuterium-ion plasma. Quantum chemistry methods might be more precise than regular molecular dynamics, but they need more computer power. So, it is hard to simulate the capacity and time frame of a system that is relevant to the plasma–material interaction (PMI). Table 1 shows the related quantum parameters used as a summary in this work. Because classical molecular dynamics uses real-world potential energy functions, making accurate predictions about a system involves a lot of thought. The programming language Python was used to run molecular dynamics simulations. This was done with version 6.0.7 of Spyder (Scientific Python Editor), which is based on the Anaconda package. The computations were done on a Dell Precision 7680 with an Ubuntu 26.04 Linux and an Intel Core i7 13th Gen processor. The Python compiler version was 3.12.7. This work used the Atomic Simulation Environment (ASE), a Python-based molecular dynamics simulation program, and PlasmaPy v2026.2.0, a Python-based plasma simulation program [8,9].

For TiB_2 crystals, lattice parameters of a = 3.028 Angstrom and C = 3.228 Angstrom, block sizes of nx = 10, ny = 10, nz = 4, and a basis of P6/mmm characterized the TiB_2 hexagonal structure. The theoretical density of TiB_2 is 59.87 g/mol, and the molar mass is 6.022×10^{23} Avogadro's number. Ten-atom deuterium plasma ions were randomly scattered 3 Angstrom above the TiB_2 lattice with kinetic energies of 40 keV to 2000 keV. Deuterium has a mass of 2.014 amu. The total number of atoms in the simulation box was

1620. The molecular dynamics simulations [7] used Velocity-Verlet. A 3T magnetic field, a 0.5 fs time step, up to 250 simulation trials, a system temperature of 513.15 K to 3000 K, and a deuterium charge of $1.6021766 \times 10^{-19}$ Coulombs were used as the simulation parameters. The simulation system used the Tersoff interatomic potential. Third-body empirical potentials like the Tersoff potential simulate Ti and B covalent bonds. Many-body interactions are based on bond order, which covers two- and three-body interactions. Two-atom bonds are considered in the Tersoff potential. A disadvantage of this approach is that the typical Tersoff potential does not have dedicated parameters for deuterium interactions with Ti and B; therefore, D was regarded as a projectile without explicit bond-order terms. Molecular dynamics simulated the beam energy and sputtering of deuterium plasma ions on the TiB_2 surface. Atoms, calculators with Tersoff, md.verlet, md.langevin, units, visualize, build with add_absorbate, velocity distribution, and optimize with QuasiNewton were the ASE modules used for the simulation. The simulation used the numpy, matplotlib.pyplot, and PlasmaPy Python modules for numerical computations, plasma behaviors, parameters, and kinetic and potential energy graphs.

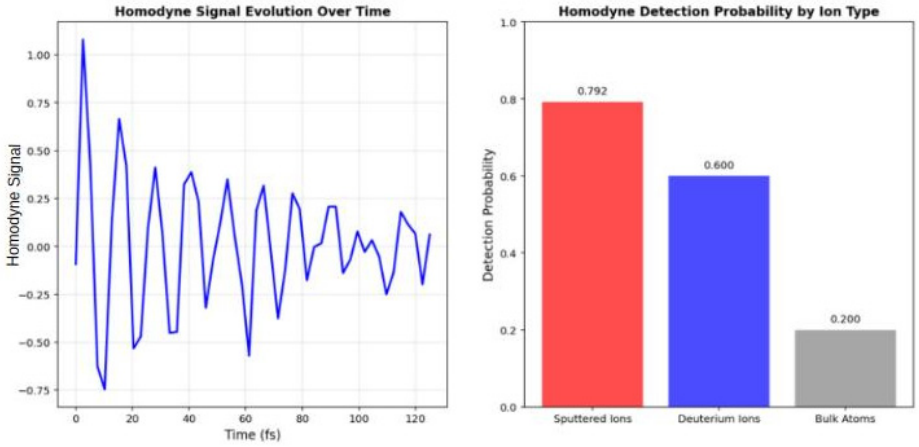
3. Results and Discussion

On the TiB_2 crystal structure, deuterium plasma ions were simulated at 40 keV to 2000 keV with a 3T magnetic field force and temperatures of 513.15 K to 3000 K. The 3T magnetic field was applied ($\vec{F} = q(\vec{v} x \vec{B})$ only to incident deuterium ions (with the help of PlasmaPy); lattice atoms experienced no Lorentz force. Next, TiB_2 bulk crystal molecular dynamics was employed. A qualitative assessment showed that sputtering may have developed as the simulation time increased. Sputtering was not observed if the simulated beam energy and temperature varied by 100 steps. Sputtering started with a higher beam intensity and temperature. The simulation system showed an unambiguous sputtering yield when the process time was extended with the deuterium-ion beam energy and temperature. During sputtering, the TiB_2 crystal deformed as the molecular dynamics process time steps increased with the beam energy and temperature. The first TiB_2 sheet layer had substitutions and voids. The TiB_2 layers were distorted enough to show deuterium atom sputtering as the simulation continued. Ten trials were conducted on the TiB_2 crystal with deuterium-ion plasma. The simulation was run 250 times with different temperatures and kinetic energies of the input deuterium ions. The sputtering yield was in the range of 0.08 to 0.21 atoms per incident deuterium ion for all the experiments. The depth profiles of the displaced Ti and B atoms showed a maximum displacement of 5–12 A below the surface. The void volume fraction increased from 2.1% at 513.15 K to 8.7% at 3000 K. The following Table 2 shows five of the 10 trials with quantum circuit analysis, and based on the five circuits, two different graphs of the homodyne analysis are presented.

The increase in entanglement entropy from 1.0986 to 1.3863 with rising temperature (513.15 K -> 1073.15 K at 40 keV) implies higher thermal disorder in the lattice and mixed contributions from quantum states in the quadrature mapping. The von Neumann entropy of the reconstructed density matrix increases with a larger thermal phonon population. The following graphs given in Figure 2 show the two homodyne plots obtained from the quantum parameters calculated and given in Table 1.

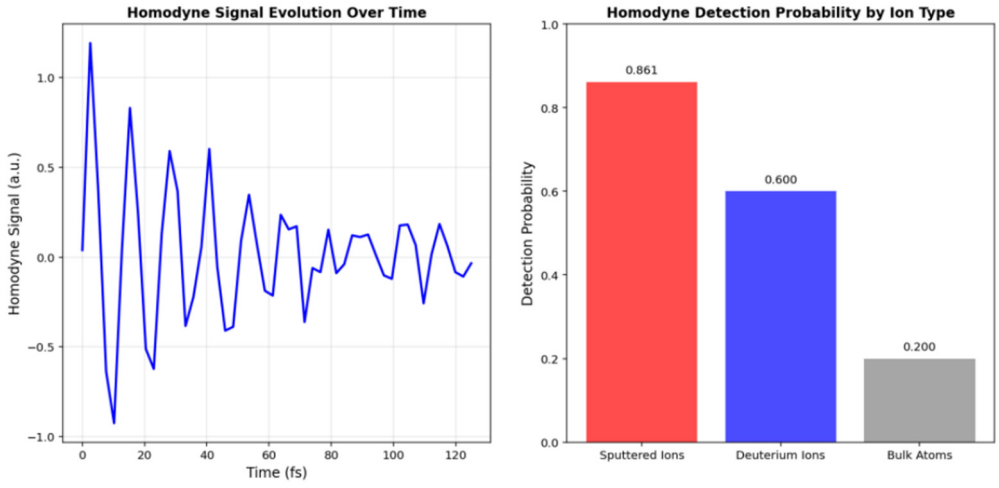
At an increased temperature (1073.15 K) and a consistent beam energy (40 keV), the sputtering efficiency increased to 0.861 (Figure 3). The molecular dynamics simulation of the TiB_2 crystal structure under deuterium plasma exposure (40 keV to 2000 keV) showed a correlation between increased beam energy, system temperature, and structural deformation. The qualitative evaluations showed increased sputtering yields and crystal defects (replacements and voids) in the primary TiB_2 crystal surface with increasing simulation length and beam intensity. The Deep Quantum platform's quantum circuit analysis indicated that quantum

quadratures affected the material's physical state. The location uncertainty increased, and the entanglement entropy increased from 1.0986 to 1.3863 as the starting system temperature increased from 513.15 K to 1073.15 K at 40 keV energy. Heat and kinetic stress on the lattice may have complicated the quantum state. At higher energy levels (150 keV and 1200 K), the mean coherence length dropped to 0.0000 Å, indicating no spatial coherence. The zero coherence length at 150 keV indicated total loss of spatial phase correlations in the quantum map, which corresponded physically to extreme lattice amorphization and destruction of long-range structural order under high-energy deuterium bombardment. High-energy sputtering and lattice disruption likely caused this. Homodyne detection signals converted physical interactions into quantum phase-space coordinates. This links continuous-variable quantum observations to classical particle dynamics.



(**a**) (**b**)

Figure 2. (**a**) Homodyne signal evolution and (**b**) homodyne detection probability by ion type for 513.15 K with ion beam energy of 40 keV.



(**a**) (**b**)

Figure 3. (**a**) Homodyne signal evolution and (**b**) homodyne detection probability by ion type for 1073 K with ion beam energy of 40 keV.

4. Conclusions

This research clearly combined classical molecular dynamics with continuous-variable (CV) quantum homodyne analysis to investigate deuterium plasma interaction with titanium diboride (TiB_2). The MD–homodyne relationship forecasted sputtering yields of 0.08–0.21 atoms/ion, and void volume fractions increased from 2.1% to 8.7+ over

513.15–3000 K. Entanglement entropy rise (1.0986 -> 1.3863) quantified thermal disorder, with the zero coherence length at 150 keV, enabling complete lattice amorphization under high-energy bombardment. Using the Atomic Simulation Environment (ASE) and Deep Quantum libraries, it was shown that the quantum quadrature operators $\hat{x}$ and $\hat{p}$ could be utilized to monitor the physical erosion and sputtering of the TiB_2 lattice. This was performed using the quantum geometry functions. The results show that increased beam energy and temperature frequently increased lattice uncertainty and entanglement entropy. Lastly, the results showed structural degradation and sputtering. According to the results, homodyne detection gives us a diagnostic instrument with a high degree of accuracy for viewing plasma–material interactions (PMIs). Moreover, it provides us with a computational framework that brings together the precision of quantum chemistry and the magnitude of classical molecular dynamics (MD). These models will be improved in the future so that they can make more accurate forecasts of the degree to which tritium will remain stable under fusion reactor conditions. Homodyne detection, moreover, provides a quantitative diagnostic for plasma–material interactions that connects quantum chemistry precision with classical MD scalability.

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Conflicts of Interest: Author Alper Pahsa was employed by Havelsan Inc. The author declares no conflict of interest.

Abbreviations

The following abbreviations are used in this manuscript:

CV	Continuous variable
MD	Molecular dynamics
A.P.	Alper Pahsa

References

1. Wojcyzkowski, K. New Development in Corrosion Testing: Theory, Methods and Standards. *AESF Found. Plat. Surf. Finish.* **2011**, *98*.
2. Kikuchi, M.; Lackner, K.; Tran, M.Q. *Fusion Physics*; IAEA (International Atomic Energy Agency): Vienna, Austria, 2012; pp. 20–21.
3. Pittard, J.A.; Fox, N.A.; Hollingsworth, A.; Lavrentiev, M.Y.; Wohlers, M.Y.; Zayachuk, A.Y. Deuterium retention in CVD diamond: Combined experimental and computational study. *Fusion Eng. Des.* **2023**, *188*, 113403. [CrossRef]
4. Kwast, H.; Muis, R.P.; Boshoven, J.G. *Tritium Retention in Neutron Irradiated Graphites, CFC's and Doped C Composites*; ECN-C--93-017; ECN: Petten, The Netherlands, 1993.
5. Jacobs, I.S.; Bean, C.P. Fine particles, thin films and exchange anisotropy. In *Magnetism*; Rado, G.T., Suhl, H., Eds.; Academic: New York, NY, USA, 1963; Volume III, pp. 271–350.
6. Whitwam, R. Scientists Design AI That Can Stabilize Fusion Reactors, ExtremeTec. Available online: https://www.extremetech.com/science/scientists-design-ai-that-can-stabilize-fusion-reactors (accessed on 12 April 2026).
7. Jun-Jie, H.; Ke-Ming, H.; Yu-Ze, Z.; Guan-Ju, Y.; Shu-Yi, L.; Xiang, Z.; Ding, W.; Fei-Xiang, G.; Ze-Feng, L.; Xiao-Wen, S.; et al. DeepQuantum: A PyTorch-based Software Platform for Quantum Machine Learning and Photonic Quantum Computing. *arXiv* **2025**, arXiv:2512.18995. [CrossRef]

8. Yorozu, Y.; Hirano, M.; Oka, K.; Tagawa, Y. Electron spectroscopy studies on magneto-optical media and plastic substrate interface. *IEEE Transl. J. Magn. Jpn.* **1987**, *2*, 740–741. [CrossRef]
9. Young, M. *The Technical Writer's Handbook*; University Science: Mill Valley, CA, USA, 1989. [CrossRef]

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