

NON-EVAPORABLE GETTER APPLICATION IN FUSION REACTORS

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ABSTRACT

Maintaining ultra-high vacuum (UHV) conditions and effectively controlling hydrogen isotopes are of great importance in fusion reactors. With the many vacuum technologies, non-evaporable getters (NEG) contribute significantly by efficiently capturing residual gases, including hydrogen isotopes. Their high, stable pumping speeds and regenerability make them ideal for integration into critical subsystems such as divertors, neutral beam injectors, and cryostats. NEG's offer distributed, passive pumping which are crucial in areas with intense plasma-wall interactions, where rapid exhaust of hydrogen isotopes, including tritium, is necessary to maintain plasma confinement and operational safety. This study builds on our previous research into advanced NEG alloys including Ti-V-Nb, Ti-Zr-V and Ti-Zr-V-Nb, aiming to identify the most radiation-resilient and high-capacity materials for fusion systems. A combined experimental-computational approach was used. Characterization techniques such as SEM-EDS, XRD and XPS evaluated surface composition and activation behavior, while density functional theory (DFT) simulations provided insights into hydrogen adsorption energetics, electronic structure (via PDOS), charge redistribution and surface bonding. To assess degradation under radiation, SRIM-based Monte Carlo simulations were used to evaluate ion implantation, sputtering yields and tritium retention depth profiles. The combined data inform predictions on NEG material lifetimes, saturation thresholds, and regeneration protocols under neutron and ion fluxes.

Keywords: Vacuum Systems, Non-Evaporable Getters, Hydrogen Isotope Management, Tritium Retention, Fusion Reactor Engineering, Radiation Damage, Surface Science, DFT

1. INTRODUCTION

Maintaining UHV and managing tritium are central challenges in fusion reactor design. NEG's offer reliable sorption of active gases without oil-based systems or moving parts. These metal alloys bind gases chemically/physically, making them suitable for high-radiation, high-temperature environments such as divertors. NEG's are effective in absorbing hydrogen isotopes (H_2 , D_2 , T_2) via reversible sorption, enabling both storage and controlled release used for tritium processing and fuel handling in ITER, SPIDER, and TFTR.

NEG materials work through two mechanisms: irreversible chemisorption for gases like O_2 , CO , and N_2 , and reversible absorption for hydrogen isotopes [1], [2]. Molecular hydrogen dissociates on the NEG surface, diffuses into the bulk, and can be released by heating ($>300^\circ C$), allowing NEG's to function as both pumps and storage beds. NEG's are used as bulk components or thin films deposited via sputtering or evaporation onto internal fusion reactor walls, ducts or diagnostics.

In practice, NEG's are implemented across fusion subsystems: divertor pumps, injectors, cryostats, glove boxes and diagnostics. Their compact, modular designs enable distributed pumping and easy integration. NEG's are especially suited to divertors handling up to 60% of exhaust and tolerating heat fluxes $>20\text{ MW/m}^2$. They maintain performance under thermal cycling and radiation for protecting plasma-facing components and minimizing gas re-ionization. In tritium fuel cycle systems, NEG's control pressure (10^{-5} - 10^{-3} Torr) and support isotope separation alongside cryogenic distillation. NEG beds are used in tritium cracking systems, removing residual deuterium before helium purification. Portable systems like LLNL's Tritium Processing System use NEG's for oil-free gas scrubbing and recovery [3], [4].

New alloy systems continue to be explored. While SAES St707 is widely used, other materials like Zr-Ni and St909 (Zr-Fe-Mn) are under study for applications in Q_{2O} reduction and tritium accounting in breeding blankets. Our research examined alternative alloys, such as Ti-V-Nb [5], using varying deposition techniques. For application in fusion reactors as tritium storage, key parameters include Sieverts' constant, embrittlement limits, operational temperature range, sorption flux characteristics, regeneration capability, sorption capacity, activation

efficiency and long-term stability.

Experimental work includes SEM-EDS (morphology, elemental analysis), XRD (crystallography), XPS (surface chemistry), surface resistance (thermal/electrical behavior) measurements for plasma compatibility. Radiation exposure studies assessed degradation, retention, and regeneration behavior under neutron and ion fluxes.

2. SIMULATION STUDIES WITH DFT AND SRIM

Density Functional Theory (DFT) simulations were employed to study hydrogen adsorption on NEG surfaces. Key outputs included adsorption energies, partial density of states (PDOS), Mulliken population analysis and electron density difference maps. These results revealed the bonding behavior, electronic modifications and preferred adsorption sites of hydrogen species on NEG surfaces, aiding in the selection of suitable alloys and defining effective activation strategies. In these simulations, optimized supercells of NEG alloys were used to model surface interactions. Exchange-correlation functionals and k-point meshes were carefully chosen to balance computational accuracy and efficiency. A range of adsorption sites and charge transfer scenarios were evaluated under different surface coverage conditions.

SRIM simulations were used in parallel to model the interactions of energetic ions (H^+ , D^+ , T^+ , He^+) with NEG materials. These simulations assessed critical parameters such as ion penetration depth, sputtering rates, and tritium retention profiles, providing insight into radiation resistance and tritium handling capabilities in fusion environments. Ion energies ranging from 1 to 100 keV were selected to replicate realistic divertor and beamline operating conditions. Key outputs from SRIM include depth-dependent energy loss, surface sputtering yields and implantation profiles relevant NEG pumps fusion energy applications. Together, DFT and SRIM simulations offer a comprehensive view of NEG material behavior under fusion-relevant operational stresses.

3. ENGINEERING CONSIDERATIONS AND SAFETY HANDLING

NEG components must be engineered for compatibility with thermal loads and diagnostics. They must endure activation cycles, saturation and temperature variations without affecting vacuum or instrumentation. Integration requires careful thermal coupling or isolation, depending on regeneration needs and should prevent cross-contamination.

NEG materials face neutron and ion bombardment, leading to helium generation, embrittlement and isotopic activation. These effects can degrade mechanical and sorption properties. SRIM modeling informs design choices e.g., material selection, shielding, and operational limits by simulating damage profiles and retention under expected reactor conditions.

NEG systems must support remote handling due to tritium uptake and activation. Their passive design allows integration into modular reactor components, enabling regeneration or replacement with minimal downtime. Compatibility with robotic systems and predefined end-of-life protocols ensure personnel safety and operational efficiency. In-situ saturation monitoring and lifecycle modeling enhance predictive maintenance.

4. FUTURE WORK AND CONCLUSION

Our integrated experimental and simulation approach supports material optimization for future systems. DFT and SRIM studies highlight promising alloy performance and guide engineering decisions under fusion-relevant conditions. Experimental data from simulated activated environments validate NEG effectiveness in tritium handling and remote maintenance. Ongoing work aims to improve radiation resistance through alloying and coatings, and to develop in-situ monitoring systems. NEGs will be key enablers of reliability and safety in DEMO-class fusion reactors and beyond.

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