

Molecular Investigations on the Diffusion of Hydrated Ions and Its Effects on the Plastic Deformation of Ultra-high Molecular Weight Polyethylene at Seawater Condition

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Abstract Ultra-high molecular weight polyethylene (UHMWPE) is a key material for marine applications owing to its outstanding self-lubrication and corrosion resistance. However, its long-term performance is compromised by plastic deformation in seawater. In this study, we performed a comparative analysis of the UHMWPE dynamics under seawater and water conditions to investigate the plastic deformation of UHMWPE induced by seawater. The results show that the plastic deformation of UHMWPE is amplified in seawater relative to the water conditions. Under thin fluid conditions, frictional interfaces exhibit a higher interfacial friction force and interaction energy in seawater than in water. Compared to freely diffused water molecules, hydrated ions occupy larger interchain spaces within polyethylene. Furthermore, the diffusion of hydrated ions weakens the interchain interactions, promoting more severe polyethylene chain rearrangement and accelerating seawater-induced plastic deformation in UHMWPE during friction. Furthermore, the diffused seawater accelerated the disentangling of the polyethylene chains and enhanced the orderly orientation distribution of polyethylene. Compared to free water molecules, the water molecules of hydrated ions exhibit enhanced attraction to free-flowing water molecules, thereby accelerating seawater flow across submerged UHMWPE surfaces. This flow enhancement promotes surface polyethylene chain mobility in seawater.

Keywords Ultra-high molecular weight polyethylene; Plastic deformation; Seawater; Hydrated ion; Molecular dynamics

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INTRODUCTION

Owing to their outstanding wear resistance, self-lubrication, and chemical stability, ultra-high molecular weight polyethylene (UHMWPE) is widely employed in aquatic mechanical systems, such as water-lubricated bearings.^[1–3] Additionally, its low density, high UV resistance, and corrosion immunity make it indispensable for deep-sea cables, anti-abrasive coatings, and other marine applications.^[4–6] Despite its favorable tribological performance as a viscoelastic polymer, the plastic deformation of UHMWPE under friction degrades its wear resistance.^[7] Plumlee *et al.*^[8] identified plastic deformation as the dominant wear mechanism in UHMWPE. Similarly, Cheng *et al.*^[9] proved that the wear of UHMWPE under seawater conditions was mainly caused by molecular chain stretching, which induced plastic deformation. Studies have suggested that incorporating graphene or inducing crosslinking via irradiation can restrict chain flow and decrease plastic deformation.^[10,11] Nevertheless, the plastic deformation mechanisms of UHMWPE in seawater environments re-

main poorly understood.

The diffusion of the molecules in the fluid film into the polymer matrix degrades the mechanical properties and leads to deformation of the interfacial polymer. Previous studies have demonstrated that the diffusion of water and squallene molecules into UHMWPE substrates reduces the flow resistance of polyethylene molecular chains, exacerbates plastic deformation, and promotes the formation of friction transfer films in our previous works.^[12,13] The ions in seawater form hydrated ions and hydrated ion clusters.^[14–16] Siriruk *et al.*^[17] calculated the water absorption rate of carbon fiber vinyl esters in seawater using the Fickian diffusion model. The results revealed that seawater saturation diffusion reduced the fatigue life of carbon fiber vinyl ester by 30%. Tribology research on fluoroelastomers (FKM) in lubricating oil (FKM-O) has revealed that competition between oil diffusion and network elastic retraction accelerates the aging-induced decline in elastic recovery.^[18]

Molecular dynamics (MD) simulations enable the atomic-scale visualization of polymer chain conformational evolution^[19–21] and fluid film rheology.^[22,23] This approach provides critical insights into the tribological mechanisms of UHMWPE in seawater systems. Cai *et al.*^[24] investigated the wear mechanisms of UHMWPE reinforced with α -zirconium

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phosphate (α -ZrP) in seawater. The MD work elucidated the load-dependent wear of UHMWPE- α -ZrP composites, which changed from extrusion deformation to adhesive wear and abrasive wear with the increase in load. Wan *et al.*^[25] demonstrated that repulsive normal forces reduce epoxy-silica interfacial friction. However, Na^+ and Cl^- ions compromise this friction-reduction effect. A parallel study documented significantly increased friction coefficients in porous α - Al_2O_3 /UHMWPE composites in seawater. The increased friction coefficients are mechanistically linked to the hydration-induced acceleration of unstable transfer film formation.^[26]

Although studies have identified the detrimental effects of seawater on UHMWPE wear, the interactions between molecules/ions in seawater and surface UHMWPE at the microscopic scale during friction remain poorly understood. This study investigated the microscale mechanisms of UHMWPE plastic deformation in a seawater environment using MD simulations. Friction systems of UHMWPE in seawater and water (control groups) environments were constructed. We discussed (i) the absorption behavior of seawater on Fe/UHMWPE surfaces, (ii) structural changes in polyethylene chains during friction in seawater environments, and (iii) seawater diffusion dynamics and the effects of diffused seawater on surface UHMWPE during friction.

METHOD

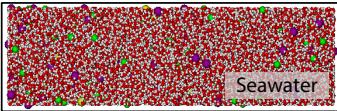
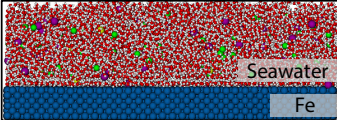
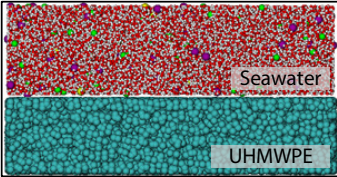
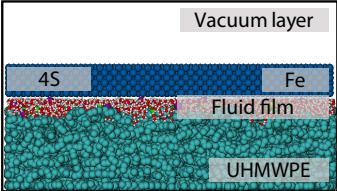
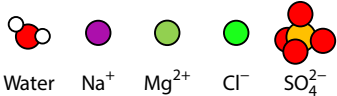
Modeling

Four types of systems, *i.e.*, ‘Liquid’, ‘S/W-Fe’, ‘S/W-UHMWPE’ and ‘4S/W, 6S/W’, are built for MD simulations. The Liquid system was conducted under the NPT ensemble for 5 ns to calculate

seawater density. The S/W-Fe and S/W-UHMWPE systems were also conducted under the NPT ensemble for 5 ns to simulate the adsorption of seawater and water on the Fe and UHMWPE surfaces, respectively. 4S/W and 6S/W systems were established to investigate the frictional behavior under the NVE ensemble. The sliding distance of the Fe plate was 2000 Å, which was 10 ns ($v=20$ m/s) and 2.5 ns ($v=80$ m/s). The detailed parameters of all systems are summarized in Table 1.

The UHMWPE plate was modeled with amorphous polyethylene,^[27] with each polyethylene chain comprising 400 carbon atoms and 802 hydrogen atoms. Litvinov *et al.*^[28] studied the entanglement properties of polyethylene with different molecular weights during the melting process. Their results showed that a polyethylene chain with a *Me* value of (1760 ± 80) g/mol, which is at least 120 carbon atoms in a polyethylene chain, can be used to describe the entanglement characteristics of the polyethylene chains. In the present work, each polyethylene contained 400 carbon atoms, which we believe was long enough to perform the entanglement state of adjacent polyethylene chains in amorphous UHMWPE. The simulation UHMWPE plate consists 24 polyethylene molecular chains with dimensions of $121.6\text{ Å} \times 82.3\text{ Å} \times 27.1\text{ Å}$ along the *x*, *y* and *z* axes. The Fe plate was modeled as a face-centered cubic (FCC) crystal structure, comprising 9384 Fe atoms with sizes in *x* and *y* directions matching the UHMWPE plate. The initial system configurations were generated using Packmol.^[29] The periodic boundary sizes in *x*, *y*, *z* directions for systems that under NPT ensemble is $121.6\text{ Å} \times 82.3\text{ Å} \times 100\text{ Å}$ in initial stage and the *z*-direction constraint is released to allow it to change during sim-

Table 1 Parameters of MD simulation systems.

System	Atomic conformation	Simulation conditions	Liquid phase inf.
1. Liquid (Density of Seawater)			
2. S/W-Fe (Adsorption on Fe)		NPT 298 K 0.1 MPa <i>t</i> = 5 ns	Water: 10000 H ₂ O Seawater: 10000 H ₂ O 0.47 mol/L Na ⁺
3. S/W-UHMWPE (Adsorption on UHMWPE)			
4. 4S/W, 6S/W (Friction)		NVE 298 K <i>t_v</i> =20m/s = 10 ns <i>t_v</i> =80m/s = 2.5 ns	4S/4W: 2000 H ₂ O (0.47 mol/L Na ⁺) 6S/6W: 3000 H ₂ O (0.47 mol/L Na ⁺)
	 Water Na^+ Mg^{2+} Cl^- SO_4^{2-}		

ulation. The periodic boundary size of friction systems which are under NVE ensemble is $121.6 \text{ \AA} \times 82.3 \text{ \AA} \times 100 \text{ \AA}$. The sizes of all systems in x , y , z -directions are sufficiently greater than the cutoff distance between unbonded atoms, which is large enough to prevent overestimation of the intermolecular interactions. Moreover, to ensure accurate force calculations in the friction systems, a vacuum layer with a thickness over 30 $\text{\AA}$ was maintained above the Fe layer to eliminate any erroneous interaction with the UHMWPE bottom surface.

We constructed two fluid film thicknesses, water and seawater, for the friction systems. The thin fluid films contain 2000 water molecules, and the fluid film thickness was 4 $\text{\AA}$. The thick fluid films contain 3000 water molecules, and the fluid film thickness was 6 $\text{\AA}$. Following standard seawater ion concentrations (represented by 0.47 mol/L Na^+) and molecular dynamics (MD) simulations of seawater,^[30] the ratio of the number of ions for all simulation systems is: $\text{Na}^+:\text{Mg}^{2+}:\text{Cl}^-:\text{SO}_4^{2-} = 20:2:18:1$. Based on the thickness and composition of the fluid films, the friction systems were designated as 4W, 4S, 6W, and 6S (4 and 6 represent the thickness of the fluid films, W for water, and S for seawater, respectively). A vacuum layer of 20 $\text{\AA}$ thickness was placed above the Fe plate in the friction systems.

Simulation Details

The Class 2 force field, employing a 9-6 Lennard-Jones potential for van der Waals interactions, has been successfully applied to model UHMWPE, demonstrating excellent agreement with the experimental surface properties and density.^[31] For water molecules, the SPC/E model, which utilizes a 12-6 Lennard-Jones potential, has been widely validated in ion solution environments,^[32] with hydrogen atom vibrations constrained by the SHAKE algorithm to maintain a rigid molecular geometry.^[33] The ions are also described by the 12-6 Lennard-Jones potential and have been verified in ion solutions.^[34,35] The interactions between UHMWPE and water/seawater were described by the 12-6 Lennard-Jones potential. The potential parameters of UHMWPE-water/seawater were employed from the work by Hirvi *et al.*^[31], which has been successfully used in polyethylene-SPC/E water droplet interfaces (simulation results show excellent agreement with experimental contact angles). These parameters have also been validated in our previous work by comparing the simulation contact angle, surface tension, UHMWPE density, etc., to the experimental results.^[12,13] An FCC model was constructed using the Lennard-Jones 9-6 potential.^[36] Consequently, a hybrid potential strategy was adopted for the UHMWPE-Seawater/Water-Fe systems. Detailed parameters are listed in Table 2. The cut-off was set at 12 $\text{\AA}$. The force field parameters are listed in Table 2. All MD simulations were conducted using the LAMMPS package employing classical force fields with periodic boundary conditions.^[37] The Lennard-Jones 12-6 and 9-6 potential formulas are as follows:

$$E = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \quad r < r_c \quad (1)$$

$$E = \epsilon \left[2 \left(\frac{\sigma}{r} \right)^9 - 3 \left(\frac{\sigma}{r} \right)^6 \right] \quad r < r_c \quad (2)$$

where E is the interaction energy between atoms, ϵ is the potential well depth, σ is the balance distance between atoms, r is the distance between atoms, r_c is the cutoff distance.

Table 2 Force field parameters.

		ϵ (kcal/mol)	σ ($\text{\AA}$)
Fe-Fe	L-J 9-6	4.79	2.64
C-C		0.05	4.01
H-H (PE)		0.02	2.99
O-O (water)	L-J 12-6	0.15	3.16
H-H (water)		0	1.78
$\text{Na}^+:\text{Na}^+$		0.35	2.15
$\text{Cl}^-:\text{Cl}^-$		0.01	4.83
$\text{Mg}^{2+}:\text{Mg}^{2+}$		0.87	1.64
S-S (SO_4^{2-})		0.25	3.55
O-O (SO_4^{2-})		0.20	3.15

The interaction energy comprises both van der Waals and coulombic contributions. Because the atomic charge of Fe was set to zero, the Fe-water interaction arose primarily from van der Waals (vdW) forces, as described by the 12-6 Lennard-Jones potential. This modeling approach is consistent with the work of Krishan *et al.*^[36], who used the same SPC/E water model and Fe parameters (Fe atom charge 0) and obtained surface energy values in agreement with experimental measurements. The work by Amin *et al.*^[38] reflected the flow characteristics and density changes of water in Fe microchannels using the Lennard-Jones potential with the atomic charge of Fe set to zero.

The above force field parameters have been verified to be applicable to water, UHMWPE, and Fe systems in a prior work.^[12] In order to verify that the force field parameters are applicable to seawater, the Liquid system (containing 10000 water molecules, 100 Na^+ , 10 Mg^{2+} , 90 Cl^- , and 5 SO_4^{2-}) is calculated through a 5 ns NPT ensemble simulation at 298 K and around 0.1 MPa. The density was determined by averaging the values over the final 1/4 of the simulation, yielding a computed result of 1.09 g/cm³. This value is very close to the experimental measurements.^[39]

The S/W-Fe and S/W-UHMWPE systems contain 10000 water molecules (S-Fe and S-UHMWPE systems containing 100 Na^+ , 10 Mg^{2+} , 90 Cl^- , and 5 SO_4^{2-}). The systems were characterized through 5 ns NPT ensemble simulations at 298 K and around 0.1 MPa, allowing the dynamics of water and seawater on the Fe or UHMWPE surface to be full time.

Friction simulations were performed using an NVE ensemble. The sliding velocities of the Fe plate were 20 m/s and 80 m/s, respectively, and the sliding distance was 2000 $\text{\AA}$. Fig. 1 shows a schematic representation of the friction simulation (taking the '4S' system as an example). For the Fe plate, a 5 $\text{\AA}$ -thick region extending downwards from the upper surface of Fe was designated as the 'v & P layer', where sliding velocity and pressure (80 MPa) conditions were applied. Conversely, in the UHMWPE plate, a 5 $\text{\AA}$ -thick region extending upward

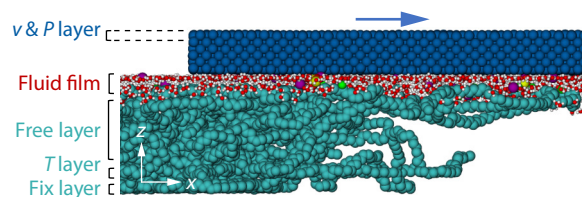


Fig. 1 Schematic diagram of the frictional configuration in the 4S model.

from the bottom surface of UHMWPE was defined as the 'Fix layer' which restricted movement in the x , y and z directions. An additional 5 Å-thick region above the Fix layer was maintained at 298 K using the Langevin method and named the 'T layer'. The free layer was defined above the T layer without any constrained dynamics. There was a fluid film (water/seawater) between the Fe and UHMWPE plates. The functions of these defined layers were comprehensively described in a previous study.^[13]

RESULTS AND DISCUSSION

Adsorption of Seawater on Fe and UHMWPE

Research has revealed that cations/anions-water molecules form hydrated ions in salt solutions.^[14] To compare strengths of ions-water (in hydrated ions) in seawater versus water-water (between free water molecules), Fig. 2(a) presents the radial distribution functions (RDF) of $\text{Na}^+\text{-O}_W$, $\text{Cl}^-\text{-O}_W$ and $\text{O}_W\text{-O}_W$ (where

O_W is oxygen atoms in water molecules) within 5 Å of Fe surface in the S-Fe system. The $\text{Na}^+\text{-O}_W$ and $\text{Cl}^-\text{-O}_W$ exhibits higher peaks than $\text{O}_W\text{-O}_W$, which decline to zero at 3 Å and 4 Å that recognized as the radius of the primary hydration shell as shown in the schematic diagrams. The highest peaks of each RDF followed the order of $\text{Na}^+\text{-O}_W > \text{Cl}^-\text{-O}_W > \text{O}_W\text{-O}_W$. This indicates that ion-water interactions are stronger than those between water molecules, and Na^+ exhibits a stronger interaction with water molecules than Cl^- . To investigate the diffusion characteristics of the liquid layer in the interface and bulk regions, Fig. 2(b) shows the mean square deviation (MSD) of O_W , Cl^- and Na^+ within both the interfacial (within 5 Å of the Fe surface) and bulk (beyond 5 Å of the Fe surface) regions. The water molecules on the Fe surface exhibited restricted mobility. Correspondingly, the diffusivity of hydrated ions in this region was also reduced. Therefore, the liquid layers are separated into an adsorbed layer and a free water layer owing to the adsorption effects. The distinct dynamical behaviors further validated the stratification of the interfa-

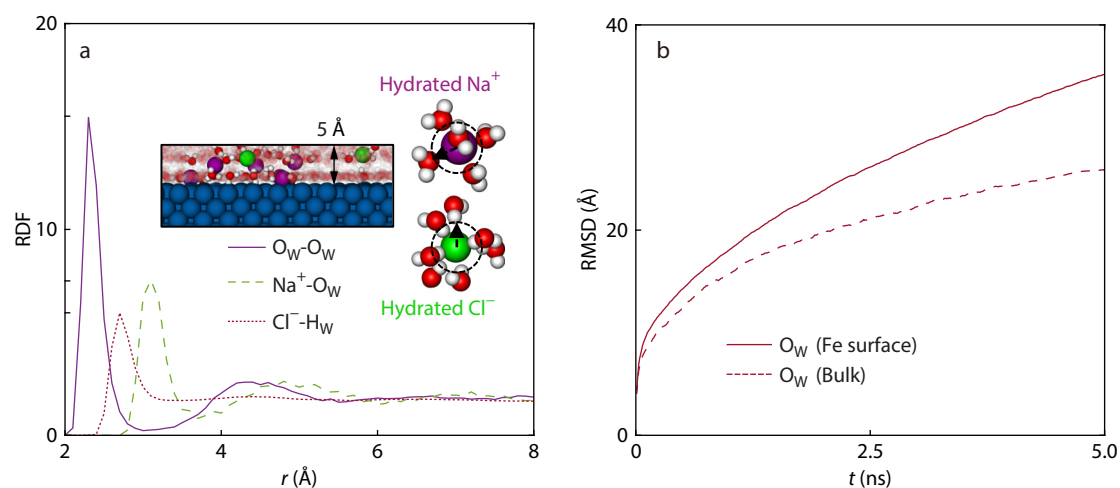


Fig. 2 (a) RDF of $\text{Na}^+\text{-O}_W$, $\text{Cl}^-\text{-O}_W$ and $\text{O}_W\text{-O}_W$ within the interfacial region (within 5 Å from the surface) of the S-Fe system; (b) MSD of O_W , Cl^- , and Na^+ in the interfacial and bulk (beyond 5 Å from the surface) regions of the seawater solution.

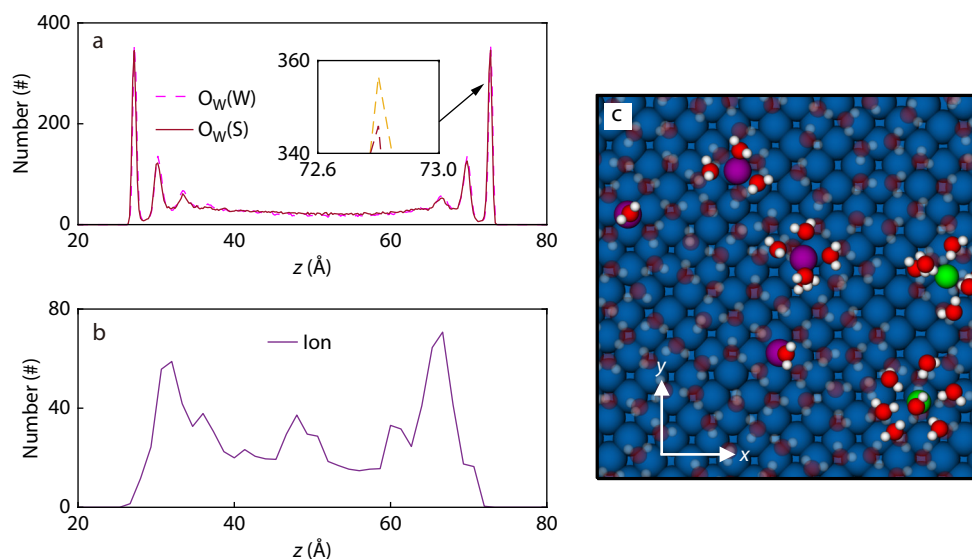


Fig. 3 Average number distribution of O_W (a) and ions (b) along z -axis over the last 1/4 process of simulation. (c) The magnified top view above 3.5 Å of Fe surfaces in S-Fe system.

cial solution structure.

To investigate the wettability of seawater on Fe, Figs. 3(a) and 3(b) show the average O_W and ion number distribution along z -axis over the last 1/4 process in the W/S-Fe systems. Both the O_W profiles of the S-Fe and W-Fe systems show pronounced peaks on the Fe surfaces, indicating the adsorption of water molecules on the Fe surfaces in both water and seawater. Comparing the O_W peaks, the S-Fe system has fewer water molecules than the W-Fe system on the Fe surfaces. The ion profile peak occurs farther from the Fe interface than the O_W peak in the S-Fe system, indicating that hydration shells prevent direct ion adsorption on Fe. Fig. 3(c) (magnified top view of above 3.5 Å of the Fe upper surface in the S-Fe system) shows that the hydrated ions are adsorbed on the Fe surfaces containing water molecules in the primary hydration shells while excluding bulk water from their inner regions. Hydrated ions occupy sites that would otherwise be available for free water molecule adsorption.

To investigate seawater adsorption on the UHMWPE surface, Fig. 4(a) displays the number distribution profiles of polyethylene carbon atoms (C_{PE}), O_W and ions in seawater of the S/W-UHMWPE systems during the final 1/4 of the simulation. The distribution of C_{PE} decreases to zero from $z=28$ Å, which defines the upper surface of the UHMWPE. Unlike the Fe interface, neither O_W nor ions exhibited distribution peaks at the UHMWPE interface, indicating negligible adsorption of water/seawater on UHMWPE. Compared to the O_W profiles, the ions exhibit higher concentrations near the midplane of the seawater film. The RDFs in Fig. 4(b) quantify the interaction strengths between the surface UHMWPE and seawater components: $C_{PE}-O_W$, $C_{PE}-O_{W-Cl^-}$ (O_W of Cl^- hydration shell), and $C_{PE}-O_{W-Na^+}$ (O_W of Na^+ hydration shell). RDF peak intensi-

ties at 3.5 Å follow $C_{PE}-O_W$ approximately equal to $C_{PE}-O_{W-Cl^-} > C_{PE}-O_{W-Na^+}$, indicating comparable interaction strengths between UHMWPE and both water molecules and Cl^- hydration-shell waters, while Na^+ ions exhibit the weakest interfacial interactions.

Interfacial Tribological Properties

The tribological properties of the friction systems were sampled within a thickness of 5 Å from the friction interface for both Fe and UHMWPE. Equal atom counts were maintained for both the materials in each computational model to ensure comparative consistency. The tribological results include the UHMWPE-Fe interfacial friction forces (F_f), interaction energies (E_{int}), and UHMWPE surface temperatures (T_{UHMWPE}). The tribological properties are averaged over the final 1/4 of the friction process and are summarized in Table 3.

To enhance the computational efficiency, sliding velocities of 20 m/s and 80 m/s were employed. However, it should be noted that variations in the sliding velocity within this range continue to influence F_f , E_{int} and T_{UHMWPE} . All systems demonstrated significantly greater F_f , E_{int} and higher T_{UHMWPE} at $v=80$ m/s than $v=20$ m/s (at $v=20$ m/s, the mild frictional conditions maintained the T_{UHMWPE} near 298 K without significant heating.). The higher F_f , E_{int} and T_{UHMWPE} values indicate that higher sliding velocities intensify friction and impede heat dissipation. At identical sliding velocities, the 6S system exhibited a lower F_f than the 6W system, whereas the 4S system showed a greater F_f than the 4W system. Both F_f and E_{int} are elevated in thin fluid-film systems.

Plastic Deformation of UHMWPE

To compare UHMWPE plastic deformation in water versus seawater during friction, Fig. 5 presents the C_{PE} velocity distribu-

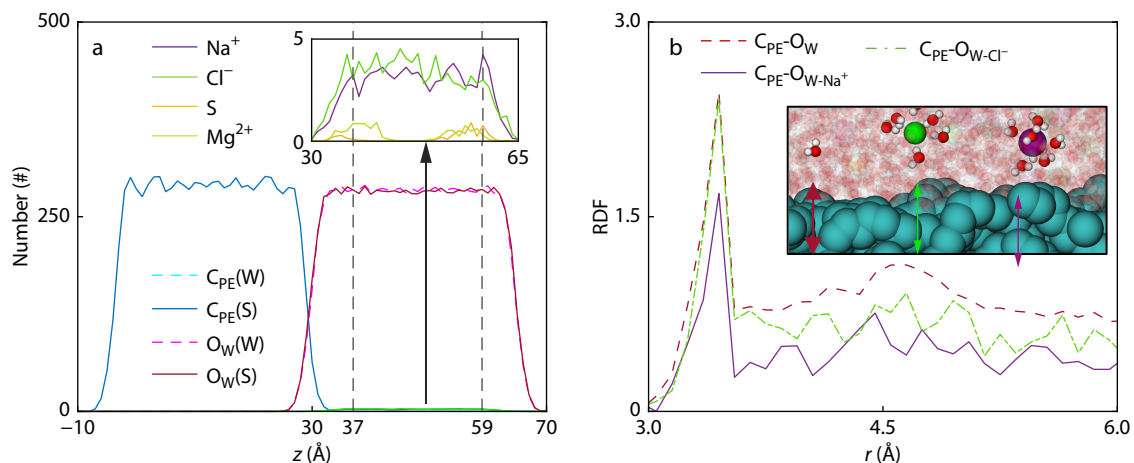


Fig. 4 (a) Average number distribution of O_W , C_{PE} and ions along z -axis over the last 1/4 process of simulation. (b) RDF of $C_{PE}-O_W$, $C_{PE}-O_{W-Cl^-}$ and $C_{PE}-O_{W-Na^+}$.

Table 3 Tribological properties of friction systems.

System	F_f (kcal/mol/Å)		E_{int} (kcal/mol)		T_{UHMWPE} (K)	
	$v = 20$ m/s	$v = 80$ m/s	$v = 20$ m/s	$v = 80$ m/s	$v = 20$ m/s	$v = 80$ m/s
4W	0.027	0.046	-235.3	-256.0	296.9	311.2
4S	0.040	0.075	-262.0	-376.6	298.4	312.4
6W	0.019	0.026	-32.9	-38.1	298.2	309.0
6S	0.004	0.007	-21.9	-28.8	299.0	311.5

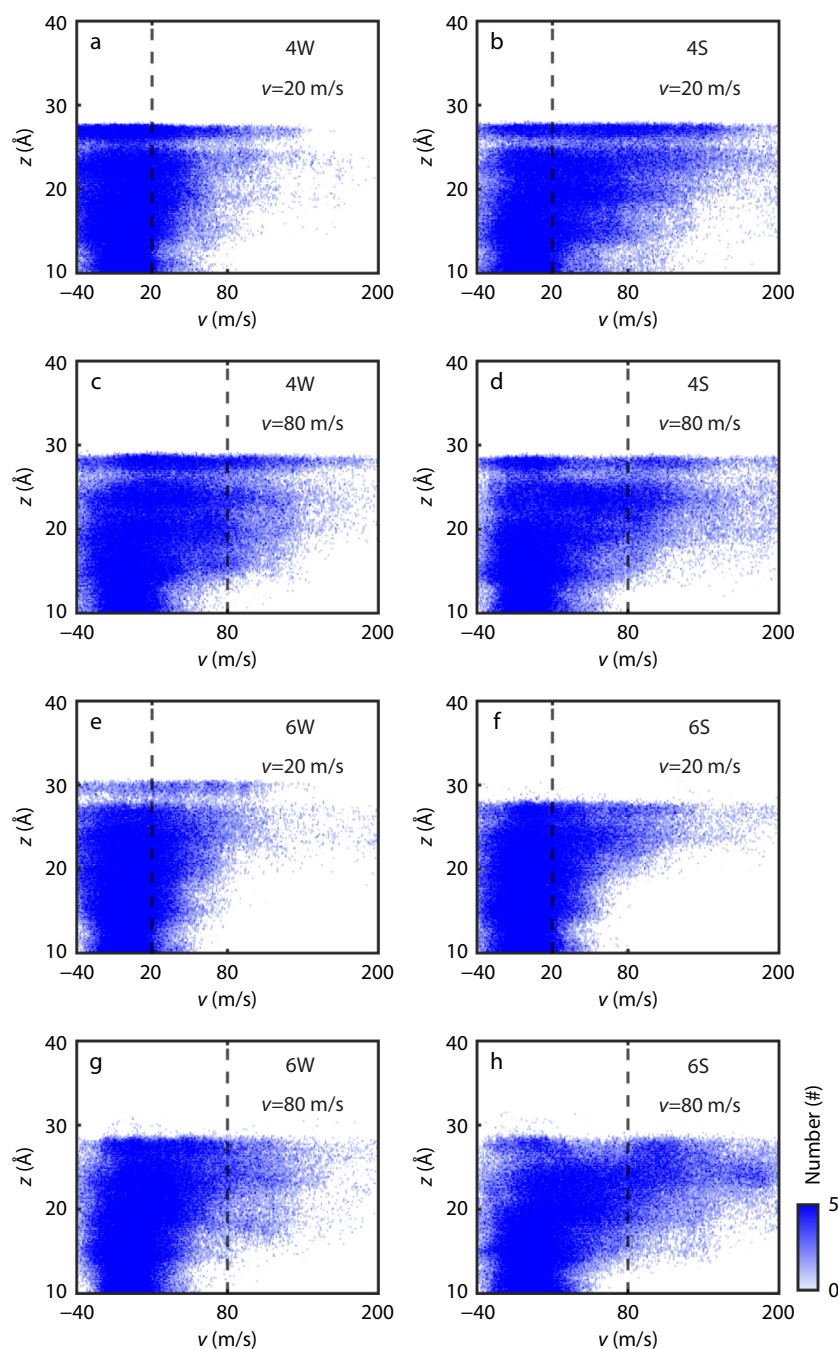


Fig. 5 The average velocity distribution of C_{PE} with sliding distance of 800–1200 Å in different models at $v=20$ m/s and 80 m/s of (a, c) 4W system, (b, d) 4S system, (e, g) 6W system, (f, h) 6S system.

tion profiles averaged over the middle stage of friction (sliding distances of 800–1200 Å). These profiles reflect the mobility of the polyethylene chains of UHMWPE during friction, where molecular rearrangement governs plastic deformation. Consequently, the C_{PE} velocity distributions quantify the plastic deformation of the UHMWPE surface.^[13] The analysis of the velocity profile revealed plastic flow in polyethylene under friction, consistent with the findings reported by Yang *et al.*^[40] The flow velocity of the C_{PE} increased markedly near the interface, corresponding to the greater plastic deformation of the UHMWPE in this region. On the other hand, at a given sliding velocity,

UHMWPE exhibited greater plastic deformation in seawater (4S) than in water (4W). Furthermore, for the same system, a higher sliding velocity results in increased deformation, as evidenced by the more pronounced plasticity observed at 80 m/s than at 20 m/s.

Fig. 6 presents molecular snapshots of the 4W/S model at a sliding distance of 1000 Å under a sliding velocity of 80 m/s. At a given sliding velocity, UHMWPE exhibited greater plastic deformation in seawater (4S) than in water (4W). The differences between the diagrams are evidenced by the more pronounced extraction of polyethylene chains in the 4S system

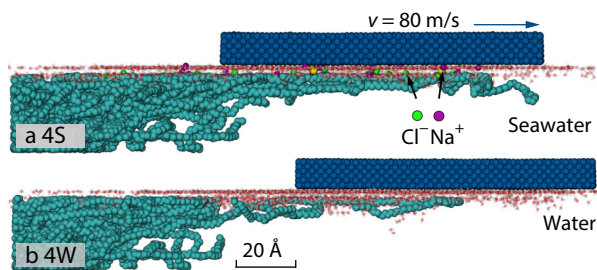


Fig. 6 Snapshots of UHMWPE of 4S (a) and 4W (b) systems under $v=80\text{ m/s}$ at sliding distance of 1000 Å .

than in the 4W system.

To investigate the evolution of the polyethylene chain orientation during friction, we computed the cosine of the angle ($\cos\theta$) between the projection onto the xy -plane of the polyethylene chain segment vector and x -axis. Each segment vector was obtained by least-squares fitting of ten consecutive carbon atoms along the polyethylene chain. The method used to calculate $\cos\theta$ is as follows.

$$\cos\theta = \frac{|d_x|}{\sqrt{d_x^2 + d_y^2}} \quad (3)$$

where d_x and d_y are the x and y components of the polyethylene segment vector, respectively.

Fig. 7 shows the variation in the distribution of $\cos\theta$ with the sliding distance in the 4W/S systems. The value of $\cos\theta$ in the 4S system was greater than that in the 4W system at the same velocity and height. Additionally, $\cos\theta$ was even greater at 80 m/s than at 20 m/s . A higher value of $\cos\theta$ indicates a greater alignment of the polyethylene segments with the sliding direction, indicating the disentanglement of polyethylene chains during friction.

The plastic deformation of UHMWPE intensifies in seawater relative to water conditions (the average velocity distribution of C_{PE} follows $4S > 4W$ and $6S > 6W$). The plastic deformation

on the upper surface was the largest, and gradually decreased as z decreased. For the same system, the plastic deformation of UHMWPE was larger at $v=80\text{ m/s}$ than $v=20\text{ m/s}$. Because the fluid film thicknesses of the 4S and 4W systems (4 Å) are thinner than those of the 6S and 6W systems (6 Å), the plastic deformations of the 4S/W systems are larger than those of the 6S/W systems.

To compare the crystallinity of UHMWPE in water and seawater environments with varying sliding distances under different sliding velocities, Fig. 8 shows the variation in the bond order parameters (S_{ij}) of C_{PE} with the sliding distance in the 4W and 4S systems. The calculation of S_{ij} is described in our previous research and is shown as follows:^[12]

$$S_{ij} = \frac{3}{2} [(e_i \cdot e_j)^2] - \frac{1}{2} \quad (4)$$

where e_i denotes the bond unit vector at atom i computed from the chord connecting its second-neighbor carbon atoms, and e_j represents the corresponding vector at atom j .

S_{ij} had a larger value in the 4S model than in the 4W model under the same velocity. Additionally, S_{ij} had the highest value in the friction surface layer and gradually decreased downwards. The higher the sliding velocity, the higher is S_{ij} . The analysis of S_{ij} reveals that plastic deformation is also reflected in the increase in UHMWPE crystallinity, with this effect being more pronounced in seawater environments. MD simulations revealed that the recrystallization of polyethylene is governed by the stretching of its molecular chains. This process becomes dominant once the chains are highly aligned along the tensile direction.^[41] Prior analyses of crystallinity elevation indicated enhanced UHMWPE wear under seawater conditions.^[9]

Fig. 9(a) shows the polyethylene chain structures at the initial and final stages of the friction process (taking the 4S system at $v=80\text{ m/s}$). Progressive plastic deformation straightens and extracts surface polyethylene chains,^[42] demonstrating deformation-induced molecular alignment. To quantify friction

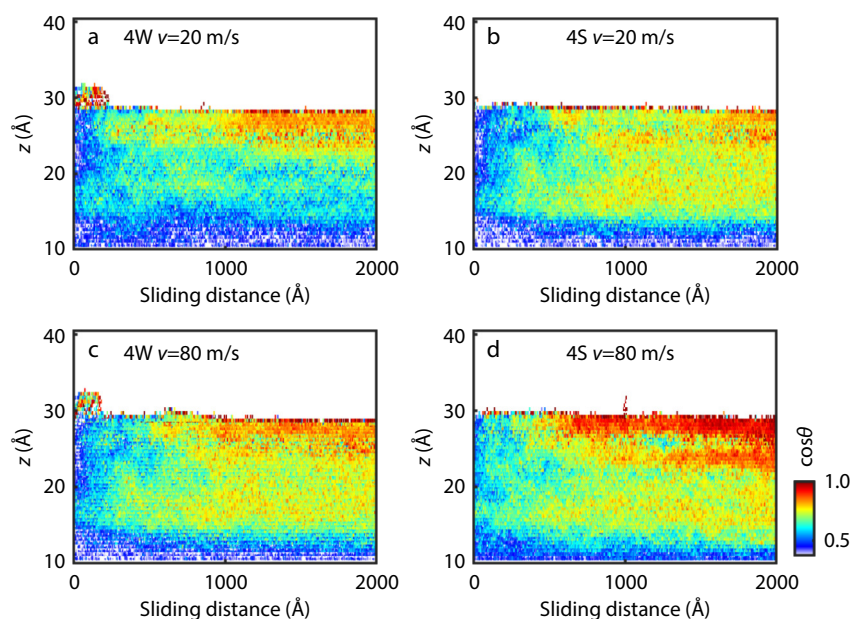


Fig. 7 variation of distribution of $\cos\theta$ in z direction with sliding distance in 4W/4S systems under $v=20\text{ m/s}$ and $v=80\text{ m/s}$.

tion-induced conformational changes in the polyethylene chains, we analyzed the flexion angles to characterize the extension and orientation of the polyethylene chains. The calculation method for the flexion angles follows that of a previous study.^[13] Figs. 9(b) and 9(c) illustrate the flexion angle evolution for polyethylene chains in 4S/W systems at $v=80$ m/s. At identical sliding distances, the 4S system exhibited a higher proportion of flexion angles $>90^\circ$ than the 4W system. This quantifies how friction induces greater polyethylene chain straightening and molecular alignment in seawater than in water environments. Research indicates that the creep deformation of UHMWPE is related to entanglement.^[43] Studies have confirmed that water diffusion into UHMWPE significantly reduces the interchain steric hindrance, resulting in polyethylene chain disentanglement.^[44] Fiber pull-out constitutes the primary failure mechanism in hybrid polymer composites (e.g., glass fiber/carbon fiber/nylon 6 sandwich structures).^[45]

Furthermore, Fig. 10(a) shows snapshots of UHMWPE, and Fig. 10(b) shows the O_W coordinate conformation at sliding distances of 200, 800, and 2000 Å in the 4W and 4S systems at $v=80$ m/s. Fluid channels and UHMWPE grooves are formed on the UHMWPE interfaces of the 4W and 4S systems. Fluid

channels and UHMWPE grooves occur because friction continuously drives the straightening of the polyethylene chain on the surface of UHMWPE. When the molecular alignment saturates, chains undergo lateral displacement, forming grooves, and allow fluid transport in channels.

The Diffusion of Seawater into UHMWPE

To compare the diffusion dynamics of seawater and water into the UHMWPE substrates during friction, the behavior of water molecules and ions in seawater was analyzed. For the water molecules, taking the thin fluid film systems as examples, Fig. 11 illustrates the variation of O_W distributions along the z -axis with sliding distances of the 4W and 4S systems. Based on Fig. 5, C_{PE} reaches a maximum z of approximately 28 Å during friction in 4S/W systems. Therefore, we conducted a focused analysis of the O_W distributions at $z < 30$ Å to discuss the diffused seawater in UHMWPE. The number of water molecules decreased at $z > 28$ and increased below them. This demonstrates the diffusion of water molecules from the fluid films into the UHMWPE substrates. Under static conditions, seawater and seawater exhibit negligible diffusion into UHMWPE, whereas friction induces diffusion of both seawater and water during sliding.

When the sliding distance is less than 1000 Å, the water molecule diffusion depth of seawater systems is shallower

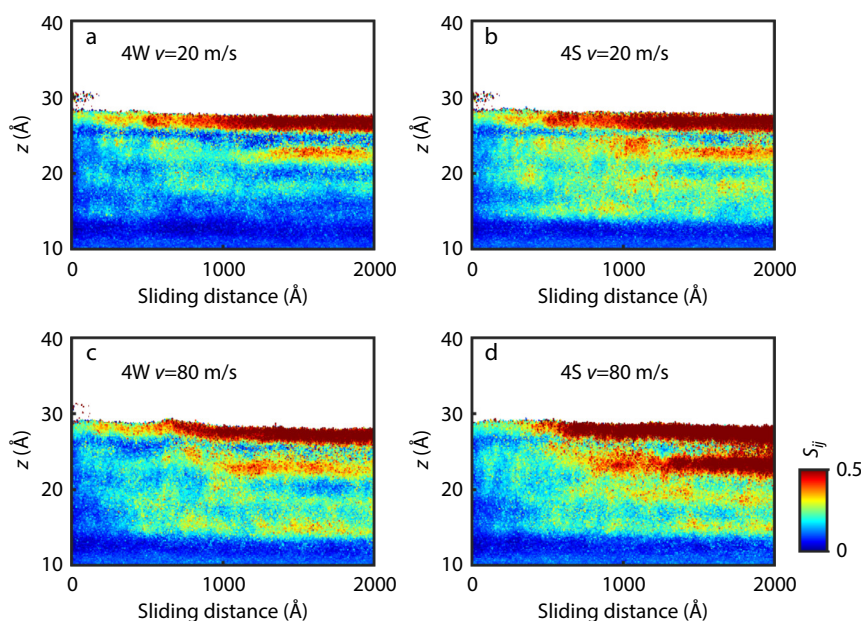


Fig. 8 Variation of bond order parameters (S_{ij}) of C_{PE} with sliding distance in 4S/4W systems under (a, b) $v=20$ m/s and (c, d) $v=80$ m/s.

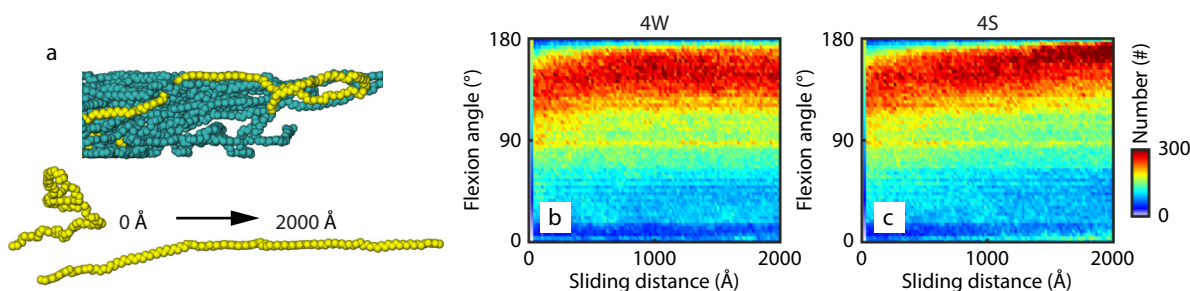


Fig. 9 (a) Schematic diagram of a polyethylene molecular chain unfolding by friction in 4S system under $v=80$ m/s; The variation of polyethylene molecular chains' flexion angle with sliding distance under $v=80$ m/s in 4W (b) and 4S (c) systems.

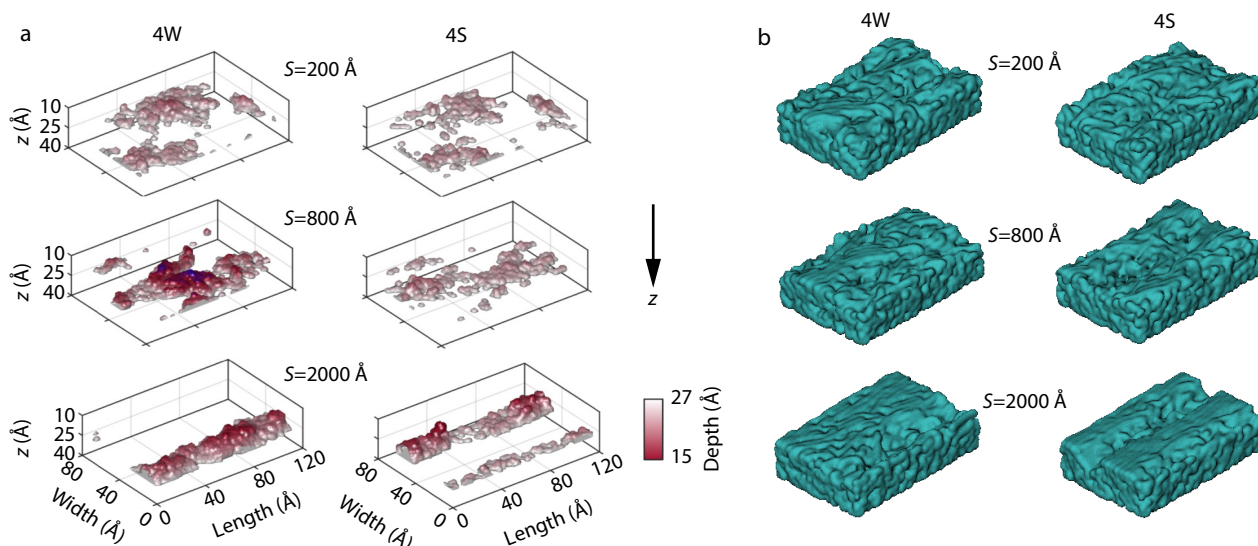


Fig. 10 (a) coordinate O_W ($z < 28 \text{ \AA}$) conformation of 4W and 4S system under different sliding distance at $v=80 \text{ m/s}$; (b) UHMWPE snapshots in the 4W and 4S systems at under $v=80 \text{ m/s}$.

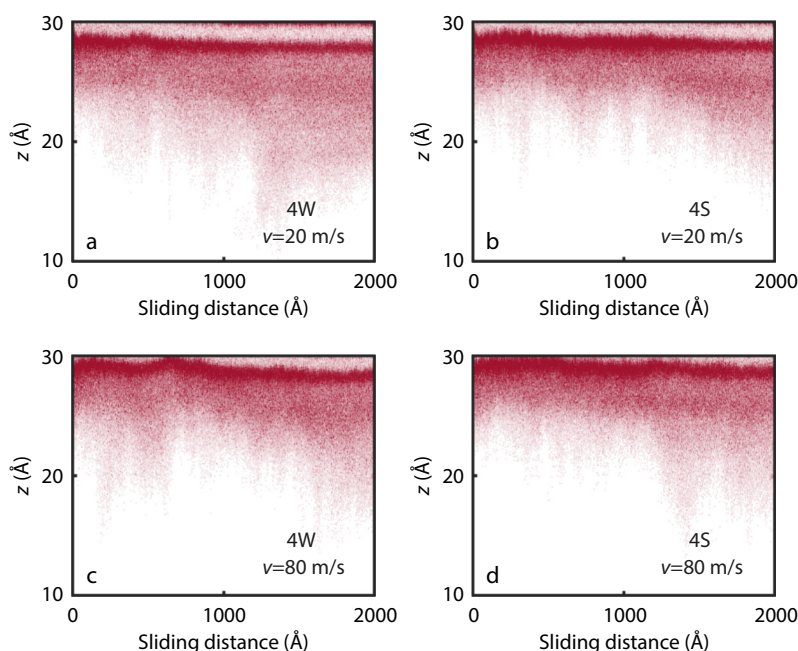


Fig. 11 Variation of O_W distributions with sliding distance of 4W/4S systems under (a, b) $v=20 \text{ m/s}$ and (c, d) $v=80 \text{ m/s}$.

than that of water systems, and the amount of diffused water molecules in seawater systems is less than that in water systems. When the sliding distance is increased to $2000 \text{ \AA}$, the depth and amount of diffused water molecules in the water and seawater systems are close. The slower diffusion of seawater into UHMWPE during the initial friction stages necessitates greater surface plastic deformation compared to water environments, primarily owing to ion diffusion effects. In contrast, seawater and water diffuse deeper under $v=20 \text{ m/s}$ than $v=80 \text{ m/s}$. Consistent with the findings of Kotelyanskii *et al.*,^[46] the W systems showed that water diffusion into UHMWPE involves expanding the plastic deformation of UHMWPE and facilitating further water diffusion. However, in S systems, the initial diffusion of hydrated ions is hindered by their large vol-

ume. As sliding proceeded beyond $1000 \text{ \AA}$, these ions progressively occupied larger interchain spaces, thereby accelerating the inward diffusion of water molecules from seawater.

In order to investigate the diffusion of ions in seawater into UHMWPE, Figs. 12(a)–12(d) present the variation of spatial distributions of Na^+ and Cl^- with sliding distance. Owing to their larger ionic radii and lower concentrations, Mg^{2+} and SO_4^{2-} exhibit negligible diffusion during sliding. Consequently, the analysis was restricted to Na^+ and Cl^- ions. Ion diffusion into UHMWPE commences at sliding distances of $1000 \text{ \AA}$ (the ion starts to distribute at $z < 27 \text{ \AA}$), where water molecules in seawater begin to diffuse into UHMWPE. Both Na^+ and Cl^- showed similar diffusion depths at the same sliding velocities. However, Cl^- exhibits significantly less distribution at $z > 30 \text{ \AA}$

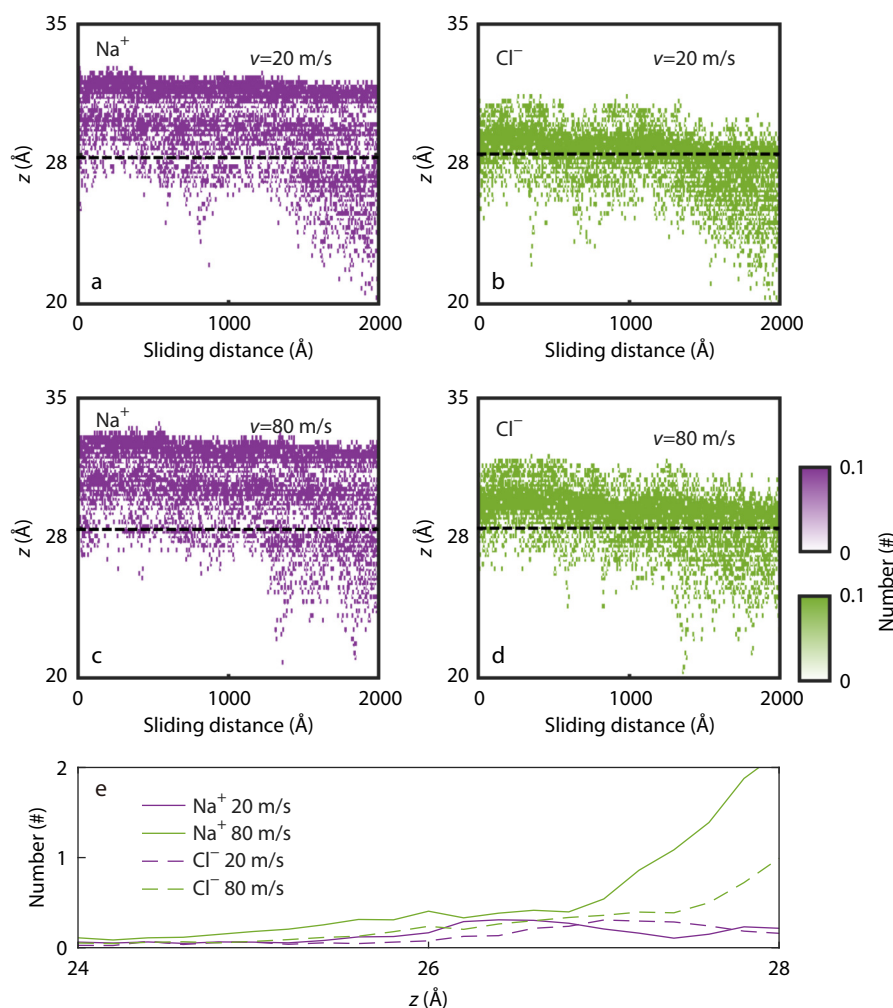


Fig. 12 Variation of number distribution of Na^+ and Cl^- along z -axis in 4S model with sliding distance under (a, b) $v=20$ m/s and (c, d) $v=80$ m/s. Average distributions of Na^+ and Cl^- over the last 1/4 friction process (e).

than Na^+ , implying less adsorption on the Fe surface of Cl^- than Na^+ . However, the diffusion depths of Na^+ and Cl^- are approximately $3.5 \text{ \AA}$ shallower than the diffusion depths of water molecules in seawater. Where the ' $3.5 \text{ \AA}$ ' corresponds to the radius of the primary hydration shell of hydrated ions, indicating that the diffused ions form hydrated ions inside the UHMWPE. Thus, the diffusion of seawater occupies large interchain spaces within the polyethylene chains because larger hydrated ions impede penetration through the polyethylene chains during the initial friction process, unlike free water molecules. Furthermore, Fig. 12(e) shows the distributions of Na^+ and Cl^- ions in the z -direction at different sliding velocities during the last 1/4 of the friction process. At a lower sliding velocity, the diffusion of Na^+ and Cl^- ions into UHMWPE ($z < 28 \text{ \AA}$) was more pronounced owing to the adequate relaxation duration during the frictional process. On the other hand, Cl^- prefers to diffuse into UHMWPE at a relatively deeper distance than Na^+ .

To investigate the impact of seawater diffusion on surface polyethylene chain interactions, Fig. 13(a) compares the average interaction energies between polyethylene chains (E_{intPE}) beyond $10 \text{ \AA}$ of the z -axis in the 4S/W systems. As the sliding

distance increased, E_{intPE} gradually decreased, with an even more pronounced reduction in the seawater environment. The decrease in E_{intPE} indicates that friction weakens the inter-chain interaction within surface polyethylene in both water and seawater environments. Furthermore, seawater exerts a greater impact on the surface polyethylene. Existing studies indicate that water molecule diffusion compromises the mechanical properties of polymers by weakening the interaction between molecular chains, as demonstrated in glass-fiber-reinforced polybutylene terephthalate.^[47]

Fig. 13(b) presents the RDF between the surface polyethylene chains ($z > 10 \text{ \AA}$) of the 4S/W systems. RDFs peaks were observed at $r_1=5 \text{ \AA}$ and $r_2=10 \text{ \AA}$, corresponding to the distances between adjacent polyethylene chains (r_1) and non-adjacent polyethylene chains (r_2), as shown in the schematic diagram. The diffusion of water and seawater induces a parallel rearrangement of the surface polyethylene chains. The lower RDF peaks at 5 and $10 \text{ \AA}$ in the seawater environment compared to those in the water environment suggest that the diffused seawater leads to a more dispersed arrangement of polyethylene chains than diffused water. A larger volume of hydrated ions (compared to free water molecules) more ef-

fectively separates the polyethylene chain. Thus, seawater diffused into UHMWPE weakened intermolecular interactions by occupying larger interchain spaces than the free water molecules.

During frictional processes, polyethylene chains undergo surface orientation changes and expulsion concomitant with molecular chain oscillations. To investigate the influence of these polyethylene chain dynamics on the diffused hydrated ions and water clusters, Fig. 14(a) shows the RDF between diffused Na^+/Cl^- ($z < 27 \text{ \AA}$)- O_W and O_W - O_W . The position and height of RDF first peaks of $\text{Na}^+-\text{O}_\text{W}$, $\text{Cl}^--\text{O}_\text{W}$ and $\text{O}_\text{W}-\text{O}_\text{W}$ in friction process are similar to that during the adsorption process. This finding is in agreement with the work of Sahle *et al.*^[48], who demonstrated the same order of interaction strength from the RDF analysis: $\text{Na}^+-\text{O}_\text{W} > \text{Cl}^--\text{O}_\text{W} > \text{O}_\text{W}-\text{O}_\text{W}$. The number of water molecules in the hydration shells remains unchanged during the friction process. Figs. 14(b)–14(g) show snapshots of the diffusion processes of hydrated Na^+ , hydrated Cl^- , and water clusters into UHMWPE over a $10 \text{ \AA}$

sliding distance. The non-deformable nature of hydrated ions causes them to sterically block and displace adjacent polyethylene chains during sliding. In contrast, water clusters always adapt to the deformation of the surrounding polyethylene chains.

Furthermore, water molecules remain stably coordinated within Na^+ hydration shells but undergo exchange in Cl^- hydration shells (Fig. 14e: translucent molecules denote initial water positions). Due to the weaker interaction between Cl^- and water molecules comparing to Na^+ and water molecules, the hydrated Cl^- ions are more prone to dissociation and reorganization with water molecules with sliding. The weaker hydrated Cl^- allows Cl^- to diffuse more readily into the UHMWPE matrix than Na^+ . Shi *et al.*^[49] indicated that in aqueous solutions containing both Na^+ and Cl^- ions, the hydrogen-bonding network around Cl^- is less stable. This observation further suggests that hydrated Cl^- ions are more prone to loss of water molecules from their coordination shells. As a result, hydrated Cl^- ions penetrate deeper into UHMWPE through con-

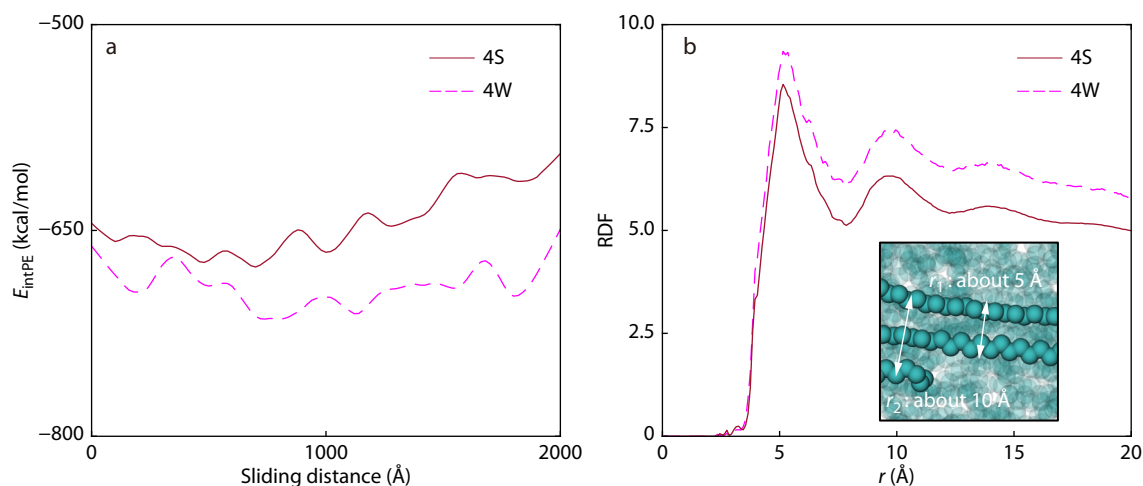


Fig. 13 (a) Variation of E_{intPE} between polyethylene chains at $z > 10 \text{ \AA}$ with sliding distance and (b) RDF between polyethylene chains at $z > 10 \text{ \AA}$ at sliding distance of 800–1200 Å in 4S and 4W systems.

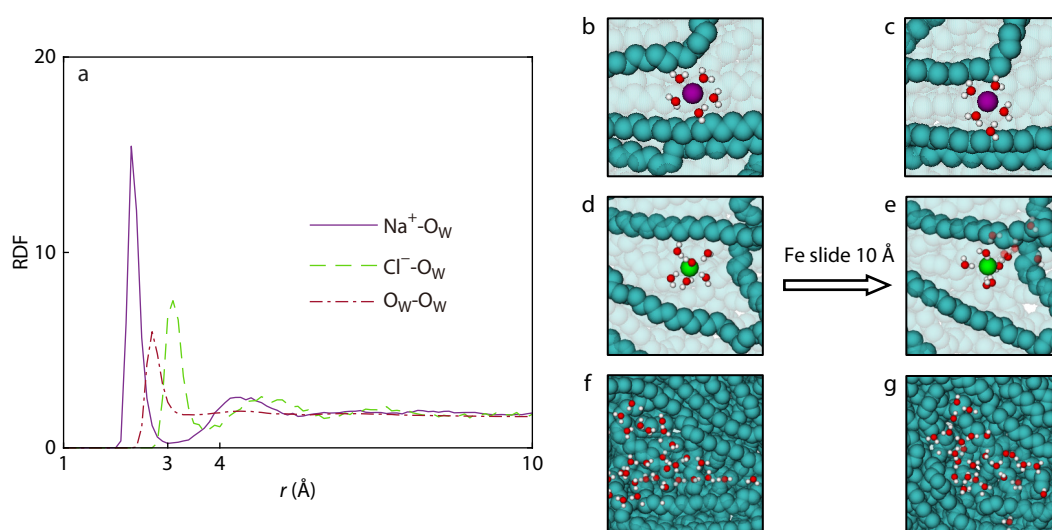


Fig. 14 (a) RDF of $\text{Na}^+-\text{O}_\text{W}$, $\text{Cl}^--\text{O}_\text{W}$ and $\text{O}_\text{W}-\text{O}_\text{W}$ in 4S system under $v=80 \text{ m/s}$. Snapshots of diffusion processes of (b, c) hydrated Na^+ , (d, e) Cl^- and (f, g) water molecules within UHMWPE over a $10 \text{ \AA}$ sliding distance.

tinuous water loss and reorganization, disrupting the inter-chain interactions more significantly and leading to greater plastic deformation. A full-atom molecular dynamics study by Ishraaq *et al.*^[50] revealed that unlike hydrated anions in bulk water, those confined within a polyethylene brush system can undergo structural reorganization to pass through the inter-chain gaps. In contrast, hydrated Na^+ ions diffused into UHMWPE as stable hydrated species. Although their diffusion is slower than that of Cl^- , they impose a stronger steric hindrance between the polyethylene chains.

To elucidate the flow behavior of diffusing seawater within the UHMWPE substrate, Fig. 15 shows the variation in the average velocities of O_W at the UHMWPE interface ($z < 27 \text{ \AA}$) with sliding distance in the 4S/W systems. The O_W velocities of 4S were higher than those of 4W. The velocity difference between the seawater and water intensified with increasing sliding velocity. The diffused seawater flows faster through UHMWPE than the diffused water, further weakening the polyethylene chain interactions and accelerating the surface UHMWPE plastic deformation.

To investigate the accelerated diffusion of seawater versus

water, we classified water oxygen atoms (O_W) into three distinct categories: (i) O_W in Na^+ hydration shells that adsorbed on Fe ($\text{'O}_{\text{W-Na}^+-\text{Fe}}'$: O_W within $3.5 \text{ \AA}$ of Na^+ which within $3.5 \text{ \AA}$ of Fe), (ii) O_W of adsorbed water molecules on Fe ($\text{'O}_{\text{W-Fe}}'$: O_W within $3.5 \text{ \AA}$ of Fe) and (iii) O_W of free water molecules (O_W). Fig. 16 shows the RDFs of 'i-iii' and 'ii-iii' in the 4S system under $v=80 \text{ m/s}$ and in the S-Fe system. The RDFs exhibited the highest peaks at $r=2.5 \text{ \AA}$. In both the 4S and S-Fe systems, the RDF peaks of 'i-iii' is higher than the RDF peak of 'ii-iii'. Hydrated ions interact more strongly with water molecules than water-water interactions in both the friction and static adsorption processes. Adsorbed hydrated Na^+ on the Fe surface enhances interactions with free water molecules, accelerating fluid film flow. This promoted the flow of diffused seawater in the UHMWPE substrate, increasing polyethylene chain separation and mobility, thereby accelerating surface plastic deformation.

The diffused seawater causes more plastic deformation than the diffused water owing to the following mechanisms: Hydrated Na^+ enlarges polyethylene chain spacing and weakens interchain interactions more effectively than free water

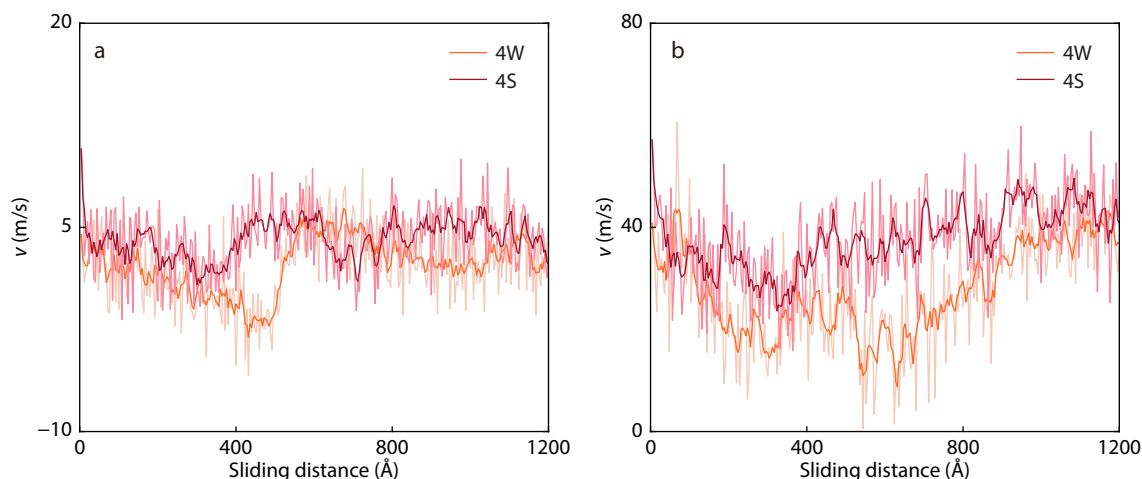


Fig. 15 The variation of velocities of O_W ($z < 27 \text{ \AA}$) in 4S/4W under (a) $v=20 \text{ m/s}$ and (b) $v=80 \text{ m/s}$.

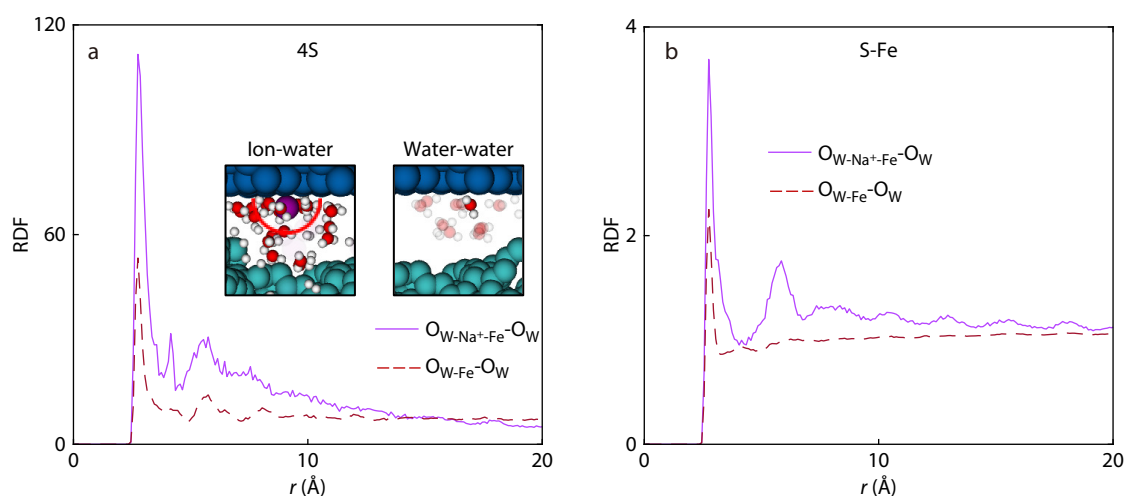


Fig. 16 RDF of " $\text{O}_{\text{W-Na}^+-\text{Fe}}-\text{O}_\text{W}$ " and " $\text{O}_{\text{W-Fe}}-\text{O}_\text{W}$ " in 4S system under $v=80 \text{ m/s}$ at sliding distance of $800\text{--}1200 \text{ \AA}$ (a) as well as in (b) S-Fe system at 1/4 part of adsorption process.

molecules and hydrated Cl^- ; Fe-adsorbed hydrated Na^+ accelerates seawater flow on the UHMWPE surface, enhancing the diffusion-driven polyethylene chains mobility and plastic deformation within the UHMWPE substrates.

CONCLUSIONS

In this study, we investigated UHMWPE plastic deformation-induced seawater diffusion and the accelerating deformation of UHMWPE by employing MD simulations. Using water systems as control groups, the wettability, diffusion dynamics, and effects of seawater on UHMWPE plastic deformation were investigated. The following conclusions were drawn: In the S-Fe system, hydrated ions are present in the seawater. The interaction strengths are as follows: Na^+ -water molecules > Cl^- -water molecules > water-water molecules. Both water molecules and hydrated ions were adsorbed on the Fe surface. In the S-UHMWPE system, the interaction between hydrated Na^+ and UHMWPE was weaker than that between hydrated Cl^- and UHMWPE, as well as free water molecules and UHMWPE. In the friction simulations, higher sliding velocities resulted in increased F_f , E_{int} and T_{PE} . In thin fluid film systems (4S/W systems), seawater environments show higher F_f , E_{int} and T_{UHMWPE} than water environments. Owing to the larger volume of hydrated ions compared to that of free water molecules, the diffusion of seawater necessitates substantial UHMWPE plastic deformation. On the other hand, the diffused hydrated Na^+ exhibits a weak interaction with UHMWPE and a stable hydration shell to increase the polyethylene chain spacing and weaken polyethylene interchain interactions during friction. The stronger hydrated Na^+ (adsorbed on Fe surfaces)-free water molecule interactions compared to water (adsorbed on Fe surfaces)-free water molecule interactions lead to faster seawater flow of the fluid film than water. The faster seawater fluid film enhanced the disturbance effect of diffused seawater on the surrounding UHMWPE and accelerated the plastic flow of the polyethylene chains of UHMWPE, thereby increasing the plastic deformation of the surface UHMWPE.

Conflict of Interests

The authors declare no interest conflict.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

ACKNOWLEDGMENTS

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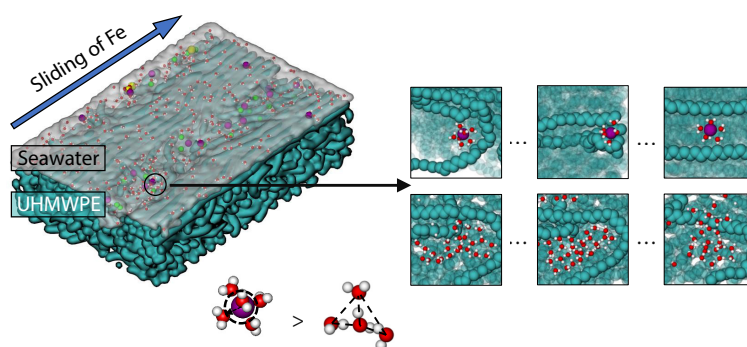
Graphical Abstract

Molecular Investigations on the Diffusion of Hydrated Ions and Its Effects on the Plastic Deformation of Ultra-high Molecular Weight Polyethylene at Seawater Condition

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Friction rearranges polyethylene chains, creating gaps. Hydrated ions and water clusters diffuse into ultra-high molecular weight polyethylene (UHMWPE) substrate, further disentangling the polyethylene chains under friction. Rigid hydrated ions exert a stronger effect than water clusters.



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