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Investigate of the Structure and Dynamics at the Water- Nickel Nanosheet Interface and Comparative by Bulk Water, with Using Reactive Force Fields

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ABSTRACT

In this work, we investigated the structural and dynamical properties of water on nickel nanosheet. The interaction of water molecules on a nickel surface was studied using reactive force field molecular dynamics (ReaxFF-MM). The results showed that water molecules near the nickel surface change in terms of structure and dynamics. The water molecules form a two-layer structure close to the nickel surface. In addition, intense stratification effects near the nickel surfaces are visible.To do so, calculations were first performed using ReaxFF in order to reproduce certain well-known properties of pure nickel and nickel-water systems. We calculated both the density profile and the radial distribution function (RDF) of the water layers from the nickel surface. The atomic probability density profile shows that water is strongly adsorbed on the nickel cristobalite surface, while the RDF indicates differently adsorbed water molecules in the first adsorption layer.

Keywords: Reactive force field; Nickel nano plate; Dynamics; Two-layer structure

1. INTRODUCTION

Surface chemistry is an emerging field that can give detailed insight about the electronic properties and the interaction of complex material surfaces with their neighbors.

This is for both solid-solid and solid-liquid interfaces. For analysis, we focused on the following properties that characterize the nickel- water interface. We calculated the density profile of the water layers from the nickel. Water is found in gas, liquid, and solid phases under ambient conditions in the biosphere and despite its simple chemical composition and structure has many unique physical properties. Many specific roles of water in biological processes have been studied, but some of its behaviors are still not completely understood [1]. In recent years, structural and dynamical properties of water in real interface systems, like water in rocks, in sandstone, and in biological

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cells have been studied [2]. Despite the simple molecular structure of water, it has unique physical properties, especially in biological systems [3].

Many experimental studies have been carried out on the water/ metal interface [4,5]. Experimental techniques such as surface force apparatus [6], differential scanning calorimetry [7], neutron diffraction [8], and nuclear magnetic resonance techniques [9] are used to study this field. The low-energy electron diffraction (LEED) method was developed in 1980 by Doering and Madey [10].

Nickel and its alloys are of numerous application due to their high potential and excellent resistance to corrosion, semi-conductivity properties, catalytic and antimicrobial activity. Their resistance against high temperature and pressure made them appropriate candidate in the nuclear industry and gas turbine engines [11].

In the present work, molecular dynamics simulations using a ReaxFF (reactive force field) were carried out with the aim of investigating the interaction of water molecules on nickel at 300 K. First, the parameters for bulk nickel were optimized. This was followed by a study of the interaction of water molecules on different nickel surfaces in order to obtain the water distribution at the waternickel interface.

2. COMPUTATIONAL METHODS

In this study, the applied nickel is three layeres with a number of 616 atoms. All MD simulations have performed with LAMMPS [12].

The structure and interaction of water molecules on Ni nanosheet, reactive molecular dynamics simulation approach was used. This technique, using ReaxFF, can calculate dynamic transfer of the charge between atoms on a nanoscale and accordingly, describes the interaction of H/O atomswith nickel [13]. Reactive force field development has been reported by Chenoweth et al. [14]. This potential has been designed to describe the chemical reactions, the dissociation and formation of chemical bonding on surfaces and etc. [15]. In ReaxFF formulation, the equation of interaction energy is a function of the bond order, which is related to the interatomic distance. van der Waals and Columbic forces are considered in this potential, as shown in equation.

$$E_{total} = E_{bond} + E_{lp} + E_{val} + E_{vdw} + E_{over} + E_{under} + E_{Coul} + E_{tors}. \qquad (1)$$

The included terms are bond energy (E_{bond}), lone-pair energy (E_{lp}), valence angle energy (E_{val}), van der Waals energy (E_{vdw}), overcoordination penalty energy (E_{over}), undercoordination penalty energy (E_{under}), Coulombic energy (E_{Coul}) and torsion energy (E_{tors}). Unlike the other terms, E_{Coul} and E_{vdw}, representative of the nonbonded terms in the equation, function independently relative to the bond order. Calculation of bond order between atoms of i and j (BO_{ij}) is in relation with the interatomic distance (r_{ij}) is shown in below:

$$BO_{ij}= exp[P_{bo1}.(\frac{r_{ij}}{r_0^{\sigma}})^{P}{}_{bo2}]+exp[P_{bo3}.(\frac{r_{ij}}{r_0^{\pi}})P_{bo4}]+ exp[P_{bo5}.(\frac{r_{ij}}{r_0^{\pi\pi}})P_{bo6}]s \qquad (2)$$

The Bond Order equation includes some parameters. In the bond order equation, r_{ij} is the interatomic distance and $r_0^{\pi\pi}, P_{bo6}, P_{bo5}, r_0^{\pi}, P_{bo4}, P_{bo3}, r_0^{\sigma}, P_{bo2}, P_{bo1}$ are corresponded to bond orders of σ bond, first π bond and second π bond, respectively.

In this section, one sheet of nickel, the applied nickel is three layeres with a number of 616 atoms, were first created using the LAMMPS package. According to the results derived from REAXFF calculations, Nickel has a face centered cubic structure (fcc) with a lattice constant of 3.511 Å. It is already consistent with the experiments. Nickel sheets were geometrically optimized, before simulation.

The initial configuration of the nickel atoms was equilibrated using a Brendsen thermostat with the relaxation parameter of 0.1 picoseconds for a period of 10 picoseconds at 300K. The periodic boundary conditions were applied only to the XY plane. Then, the structure is simulated in NVE ensemble for 10 picoseconds. Thermodynamics properties as total energy and temperature have been monitored to examine the process of equilibration. TIP4P/ice potential model was used to describe interatomic and intra-atomic energy interactions for water molecules. This model predicts the density of liquid water as 993.0 gr/cm^3 at standard conditions (298 K and 1 atm) which is consistent with the experimental density of 997.0 gr/cm^3. Integration of the motion equations is performed using Verlet algorithm with time step of 1 femtosecond. In addition, 566 of water molecules randomly filled on the nickel surface. The system is equilibrated in the NVT ensemble for 1 nanosecond at 298.15 K via Nose-Hoover thermostat with the relaxation time of 1 picosecond. Then, the simulation continued for 10 nanoseconds in micro-canonical ensemble (NVE). Noteworthy, density calculation of water is performed in the z-axis direction perpendicular to the nano-sized surface.

3. RESULTS AND DISCUSSION

In order to determine the structure of water molecules on the nickel surface, the density profile of water molecules was calculated. Further studies were done by calculating the orientational ordering, radial distribution functions.

3.1. Density Profile

Density profile of the oxygen atoms in the water molecules on the sheet of nickel are shown in Fig. 2a.And the peaks have high intensity near the nickel surfaces. This indicates the stratification effects close to the nickel surface so the density of layer near the surface possesses higher values relative to the center. The first two peaks indicate that two layers of water are formed near the nickel surface, which these two layers show a higher density than the center. These results are consistent with previous studies. The first adsorbed layer of water is observed at a distance of 2 Å from the surface. This result is different from the results obtained by Van Duin et al.,

3.2. Radial distribution function

Radial Distribution Function (RDF) is a valuable criterion for describing the structure of water close to the surface. The radial distribution functions of oxygen-oxygen and oxygen-hydrogen are shown for the water molecules on the nickel sheet and bulk water .The RDFs of the bulk water were also plotted at 298 K. These plots have been compared in Figure 3.

The radial distribution function of nickel-hydrogen and nickel-oxygen are plotted for the three layers at different distances from the nickel surfaces in Fig. 4 surface and Layer 3 is the Middle layer.

The radial distribution function of nickel-oxygen represents a sharp peak at a distance of 2Å. The distance of the peak is approximately same as 1.9Å, which is very close to the length of the bond reported . In addition to the first peak, a peak with lower intensity is also observed at 4.2 Å. It is related to the distance of the second neighbor of water molecules near the surface.

4. CONCLUSION

The results demonstrate that for nickel

surface, water molecules are adsorbed in the form of a bilayer structure. The first layer is located at a distance of approximately 1.0 Å from the surface nickel atoms, in a configuration where the dipole moment of water is perpendicular to the surface. The second water layer is located at a distance of 2.0 Å from the surface nickel atoms, and the molecules are held to those of the first layer by hydrogen bonds.

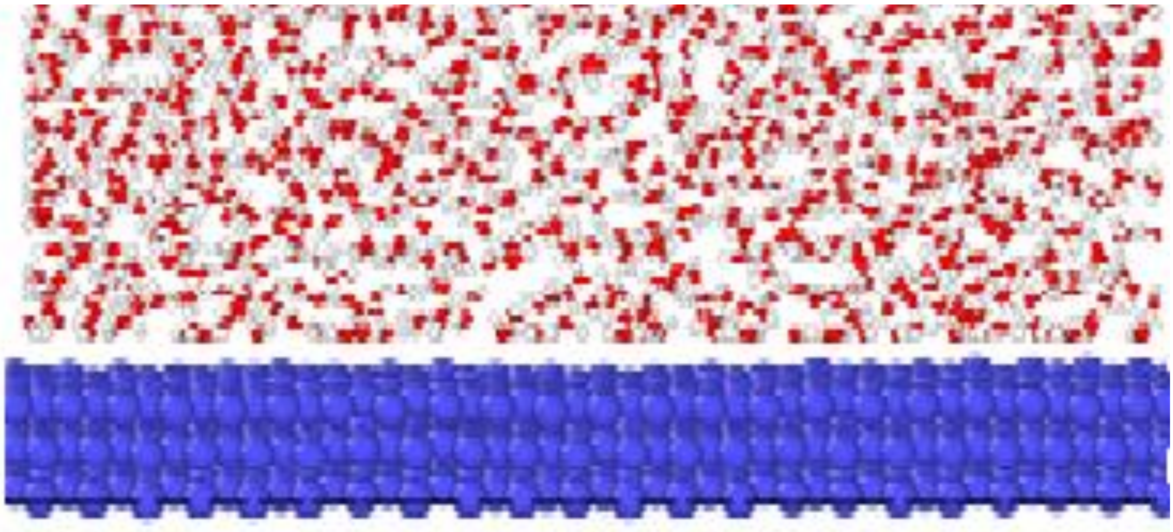


Fig. 1. Initial configuration of water on the nickel nanosheet. O, H and Ni are presented with red, white and blue, respectively.

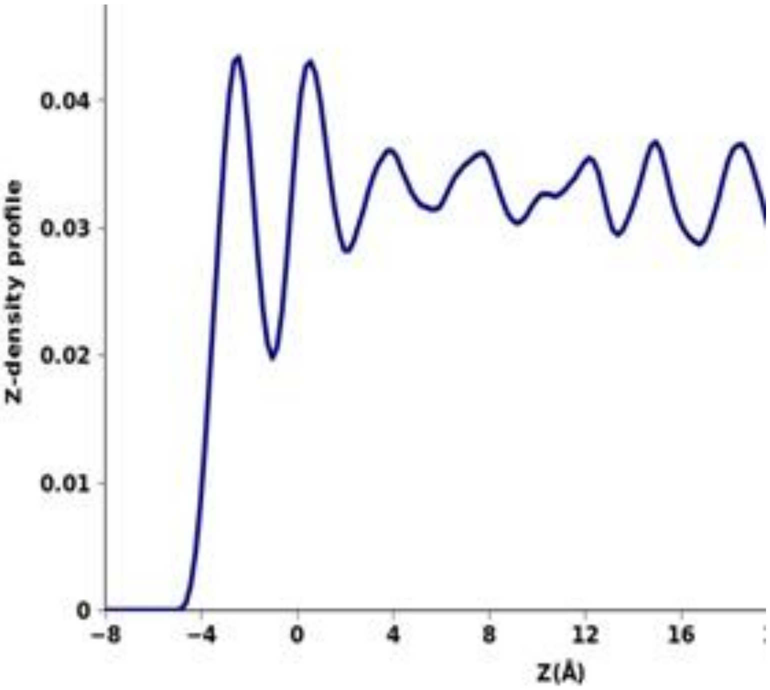
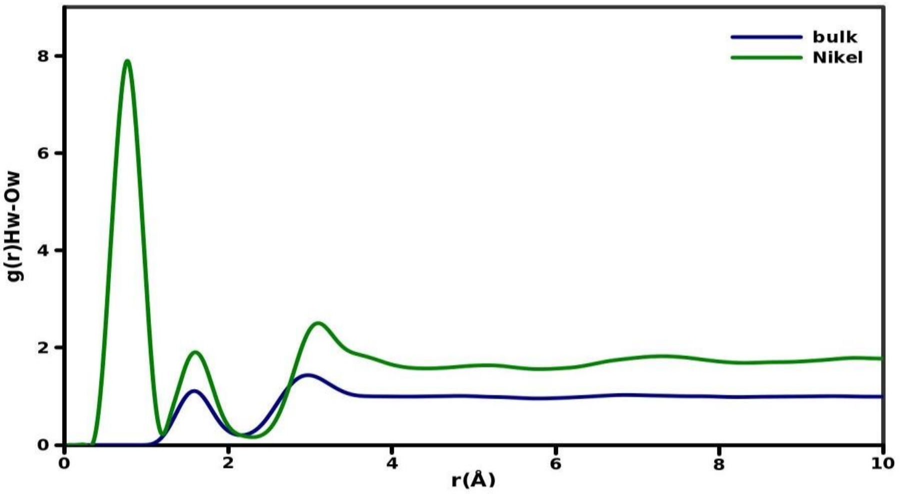


Fig 2. Density profile of oxygen atoms in the water molecules on the surfaceof nickel along z.



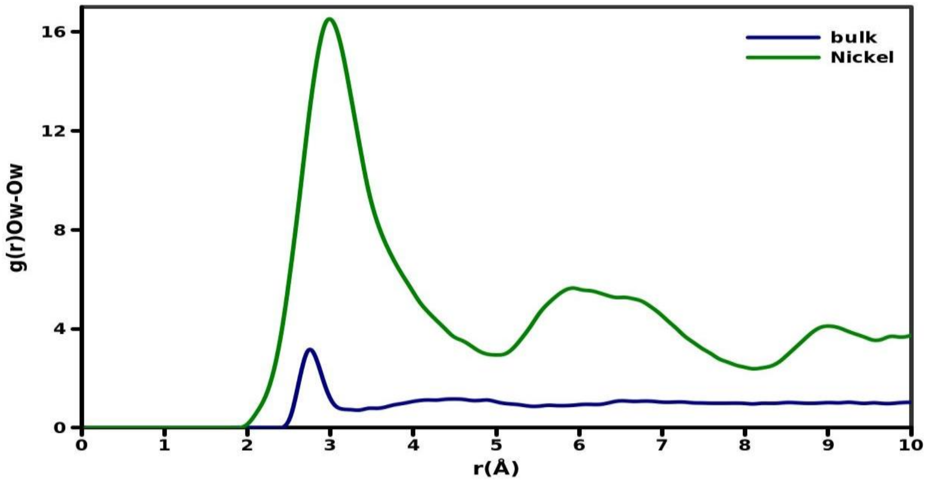
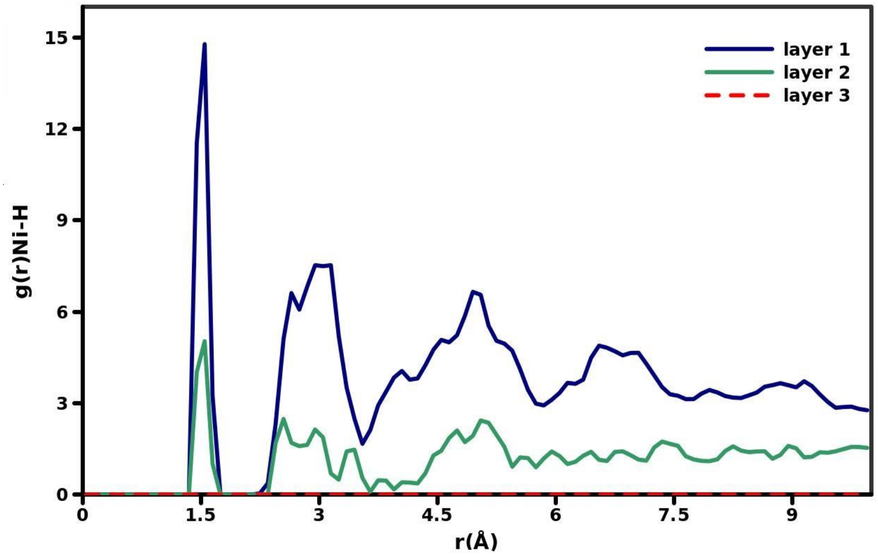


Fig .3. a) O-O RDF b) O-H RDF of water molecules confined between nickel surfaces. Close layer of confined water molecules and bulk water are plotted.



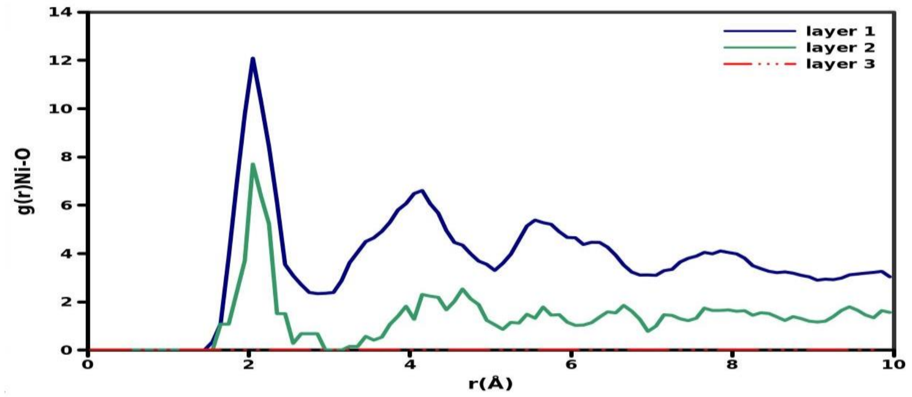


Fig .4. a) Ni-H RDF b) Ni-O RDF of molecules on the nickel surface. Layer1 and Layer 2 are layers close to the surface and Layer 3 is the Middle layer.

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مجله شیمی فیزیک و شیمی نظری
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بررسی ساختار و دینامیک سطح مشترک آب- صفحه نانو نیکل و مقایسه آن با آب توده ، با استفاده از میدان های نیروی واکنش پذیر

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چکیده

در این کار، ما خواص ساختاری و دینامیکی آب را روی نانو صفحه نیکل بررسی کردیم .برهمکنش مولکول‌های آب بر روی سطح نیکل با استفاده از دینامیک مولکولی میدان نیروی واکنش‌پذیر مورد مطالعه قرار گرفت. نتایج نشان داد که مولکول‌های آب نزدیک سطح نیکل از نظر ساختار و دینامیک تغییر می‌کنند. مولکول‌های آب یک ساختار دو لایه نزدیک به سطح نیکل تشکیل می‌دهند. علاوه بر این، اثرات لایه ای شدیدی در نزدیکی سطح نیکل قابل مشاهده است. برای انجام این کار ، ابتدا محاسبات با استفاده از میدان نیروی واکنش‌پذیر به منظور بازتولید برخی از خواص شناخته شده سیستم‌های نیکل خالص و آب نیکل انجام شد. ما مشخصات چگالی و عملکرد توزیع شعاعی لایه‌های آب را از سطح نیکل محاسبه کردیم .مشخصات اتمی تابع چگالی نشان می‌دهد، که آب به شدت بر روی سطح نیکل کریستوبالیت جذب می‌شود، در حالی که توزیع شعاعی مولکول‌های آب جذب شده متفاوت را در اولین لایه جذب نشان می‌دهد.

کلید واژه‌ها: میدان نیروی واکنش‌پذیر؛ نانو صفحه نیکل؛ دینامیک، ساختار دو لایه

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