Polystyrene nanoparticles as a flotation collector: A molecular dynamics study

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Abstract

Nanoparticles have significant potential as new candidates for generating new types of flotation reagents with unique performance for wettability design and control. Hence, this study explores the wettability of a glass surface covered with polystyrene nanoparticles at various surface coverage percentage using molecular dynamics simulations. To investigate wettability on the bare and coated glass surface, the dynamics of water molecules, contact angle, density distribution profile, and hydrogen bonding patterns are analyzed as substrate wettability indicators. The results reveal that both unrelaxed and relaxed forms of glass surface tolerate a strong asymmetric distribution of surface energy in general, due to charge accumulation on the surface leading the surface to strong hydrophilic behavior. However, unlike chemical collectors, partial covering of glass surface with cationic polystyrene nanoparticles up to 10% reduces the surface tension to a favorable level of hydrophobicity for flotation.

1. Introduction

Flotation [1] is one of the most important and widely used methods in mineral and material processing [2]. Increasing demand for raw material has caused a greater need to use low grade [3], and complex mineral resources [4], recycling of materials [5] and recovery of minerals from fines [6]. Moreover, increasing environmental problems, which are associated with using industrial chemicals [7] along with the foregoing description make it inevitable to look for a new and more efficient generation of flotation reagents with the possibility of recycling and reuse. Among new ideas, nanoparticles are one of the most interesting and promising alternatives for common chemical reagents due to a series of extraordinary features such as the possibility of synthesis in a wide range of dimensions, several synthesis methods, increased surface area, easy detachment, easy recycling capability, low environmental issues compare to chemicals, and ability to physical adsorption [8].

The potential of nanoparticles for these applications has promoted substantial interest and work on the reagent performance using nanoparticles as flotation reagents. Hajati et al. [9] studied the application of talc nanoparticles as a collector in quartz flotation. Their outcomes indicated that it is possible to replace chemical collectors with hydrophobic talc nanoparticles for quartz flotation. Cao et al. [10] examined graphene oxide for de-sliming of super-hydrophilic serpentine coating in pentlandite flotation. Pelton et al. [11–17] started a series of fundamental studies on using stabilized hydrophobic nanoparticles as a collector in flotation. They successfully replaced chemical collectors with hydrophobic polystyrene nanoparticles in glass and pentlandite flotation affected by thin layer coating of hydrophilic fines and ions. Adsorption of hydrophobic polystyrene nanoparticles on hydrophilic mineral surface is found to lead to a significant change in the surface wettability and enhancement in the performance of the hydrophilic mineral flotation.

In this work, we particularly investigate adsorption phenomena and hydrophobicity of mineral surfaces from a molecular point of view. Considering acceptable results of simulation and modeling methods based on quantum mechanics [18–22] and molecular dynamics simulations [23–30] in the similar cases, Molecular Dynamics (MD) is used for investigating inter and intra-atomic interactions among polystyrene nanoparticle, silicon dioxide (glass) surface, and water molecules. Specifically, we study effect of polystyrene nanoparticles on interactions between water molecules and glass (001) surface by using classical molecular dynamics. Wettability on the bare and coated glass surface with polystyrene nanoparticle in various surface coverage percentage is discussed with contact angle, diffusion, and hydrogen bonding phenomena. The process of adsorption, formation of water nanodroplet, and pinning for water nanodroplet and polystyrene nanoparticle are also discussed.

2. Computational details

Fig. 1-I and Table 1 present the model and configuration details on six systems used in this work to perform the MD simulations. A glass-
water system (GW) is used to investigate the wettability of a bare glass surface. Glass-polystyrene-water (GPW) systems with five (GP05), seven (GP07), and ten (GP10) percentage of surface coverage are used to analyze the relation between surface coverage percentage and changes in the surface wettability. A GPW model with two smaller nanoparticles instead of one larger nanoparticle in the same surface coverage percentage (G2P05) is used to investigate the effect of nanoparticle size on surface wettability. To investigate the effect of substrate termination on wettability, a GPW surface with silicon termination (GsP10) is used to compare with the case of oxygen termination.

Fig. 1. (I) Initial configuration of simulation systems, (II) atom types for Atactic polystyrene chains.
(GP10). The dimensions of the glass surfaces in the molecular models are $151 \times 151 \times 21\,\text{Å}^3$ in the x-, y-, and z-direction, respectively.

To create stabilized polystyrene nanoparticles with desired sizes and density (1.04 g·cm$^{-3}$), polystyrene chains in Atactic tacticity are initially packed into amorphous cells with the structural details described in Table 1. The simulation cells are then subjected to an annealing process to create the bulk aggregation of polystyrene, and are simulated with the constant-temperature, constant-pressure (NPT) ensemble at a temperature of 300 K and ambient pressure [31]. The atom types used for the modeling of styrene chains are shown in Fig. 1-II. To simulate the water nanodroplets, water amorphous cells including 1000 of water molecules are constructed with the dimensions of $35 \times 35 \times 35\,\text{Å}^3$ in the x-, y-, and z-directions.

To eliminate edge and boundary effects, the water cells and the polystyrene nanoparticles are located in a distance of more than 25 Å with respect to the glass edges of the simulation boxes. To minimize the direct repulsive effect of polystyrene nanoparticles on water nanodroplets and on its contact angle, the water and the nanoparticles cells are located on the opposite sides of glass surface at a distance of more than 20 Å. The water cells are located on the down left side of glass surface while the nanoparticles are located on the top right side of the glass surface in order to mitigate any effects of surface geometry on contact angle (Fig. 2). The periodic boundary conditions are considered in the x- and y-directions only while non-periodic boundary condition is considered in the z-direction due to the physics of system.

The MD simulations are performed using the open-source code Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [32]. Visual Molecular Dynamics (VMD) [33] is used for visualization of structures and post-processing of simulation data. The Consistent Valence Force Field (CVFF) [34] is used to describe the intra and inter atomic interactions (Table 1). Due to greater compatibility with the CVFF parameters, water is described with the TIP3P [35] potential energy model. The 6–12 Lennard-Jones potential energy model [36] is used to model all non-bond interactions. Particle, Particle, Particle, Mesh (PPPM) algorithm [37], a Fourier-based Ewald summation method, is applied with the tolerance of $1 \times 10^{-4}$ to include the long-range electrostatic interactions. The Verlet algorithm [38,39] is used to integrate equations of the motion in the simulation boxes. During the simulations, the glass surfaces are considered fixed at their initial position. A time step of 1 fs is used for all simulations. The simulations are carried out for 5 ns in the constant-temperature, constant-volume (NVT) ensemble using a Nose-Hoover thermostat [40] to keep the temperature at 300 K.

3. Results and discussions

3.1. Surface tension

Adsortion, configuration, and mobility of water molecules on a solid surface are significant reflections of physics and chemical nature of the surface atoms and molecules. In other words, surface energy plays a significant role in wettability behavior and properties and investigating its origins and distribution will provide a better understanding of the wettability properties of the surface. To assess the origin and the quality of the energies distribution on the glass (0 0 1) surface, energy analyses [41] are performed for both unrelaxed (terminated with O radicals) and relaxed forms (terminated with Si radicals) [42] of the glass surface. To record the distributions of Coulomb, van der Waals, and total energies on the glass surface, based on the density distribution profile of water molecules on the bare glass surface (Fig. 7), one water molecule is located at an equilibrium distance with respect to the glass surface to scan it. During this process, the non-bond interactions between the water molecule and the surface are calculated.

Using the glass surface as a reference for the energy distributions reveals that the minimum values for Columbic energy in both forms of glass surfaces occur at the inner core of the glass surface compared to the edge regions due to the lower density of incomplete SiO$_2$ structures. In addition, by moving toward the edges, the distribution of Columbic energy shows non-uniform incremental trends due to asymmetric structure of the glass. Hence, depending on the density, presence, and positioning of free radicals, different distributions of Columbic energy are observed on the edges. Van der Waals energies show a more uniform distribution as well as lower variations. Total energy at any place on the glass surface is equal to the sum of Columbic and van der Waals energies. Compared to Coulomb contributions, the van der Waals energy is relatively small; therefore, the total energy on both terminations of glass surface is dominated by the Columbic energy. The total surface energy on the relaxed glass surface is also lower than the one on the unrelaxed glass surface, which is expected, but it shows that the location of free oxygen radicals with respect to glass surface has a higher significant effect on surface tension.

Generally, the energy analysis results on the possible terminations of the glass surface show that despite a significant difference in values of surface energy on these surface arrangements, it is of the same nature resulting from accumulated partial charges, especially located at the edges due to dense presence of incomplete Si—O bonds. This strong accumulation of surface tension allows the glass surface to strongly adsorb cationic ions and polar water molecules, reorienting them toward the surface, forming hydrogen bonding with water molecules, and thus becoming strongly hydrophilic. The results are in good agreement with other works found in the literature [43].

3.2. Stability of the adsorption systems

To determine the contact angles from MD simulations, it is necessary to make sure that the structure remains stable and fixed on the glass surface. In the following subsections, we present analysis and results on the stability of adsorbed nanoparticles and formed nanodroplets further, before contact angle calculations.

3.2.1. Stability of the adsorbed nanoparticles

In MD simulations of bio-molecules, polymers, and long-chains, the root-mean-square displacement (RMSD) [44] represents a measure of...
the average distance of molecules and/or atoms among structures or clusters. Hence, a steady value of the RMSD also indicates that the system has reached equilibrium conditions. Fig. 2 shows RMSD values for carbon atoms in polystyrene nanoparticles and hydrogen atoms in water molecules. As seen in Fig. 2-I, due to strong electrostatic interactions, the nanoparticles adsorb to the glass surface and reach to equilibrium conditions at the initial stages of the simulation.

To verify pinning of nanoparticle on the glass surface, the location of center-of-mass (COM) of adsorbed nanoparticle is monitored in the x- and y-directions. Fig. 3 shows steady values of COMs in different simulated systems. The steady positions of COMs in the x- and y-directions confirm stable positioning of the adsorbed nanoparticles on the glass surface due to strong electrostatic interactions.

3.2.2. Stability of the formed nanodroplets

Stability analysis of formed water droplets is important in particular for calculation of contact angles and wettability analysis. Fig. 2-II shows RMSD values for hydrogen atoms in water molecules of various simulation systems. These reveal that water molecules interact with the glass surface and polystyrene molecules, and converge to equilibrium approximately after two nano-seconds, indicating the formation of nanodroplets and their respective equilibrium structures. The results also show that on the glass surface the process of adsorption and stabilization of polystyrene nanoparticle is faster than the process of water molecules adsorption and nanodroplet formation.

Mean-square displacement (MSD) [45] is an indicator of mobility and movement for water molecules in the immediate contact with a
solid surface. The convergence of MSD of water nanodroplets on a surface indicates that the process of their formation is complete with stable shape and contact angle on the surface. Fig. 4 shows MSD values of water molecules as a function of time. The GW label is the results for MSD of water molecules on the bare glass surface. Due to the strong electrostatic interactions at the beginning of simulation, a sharp ballistic motion of water molecules is observed. Water molecules with fast movements are readily adsorbed on the glass surface. Strong hydrogen bonding forms between hydrogen atoms of water molecules present in the interface and oxygen atoms of glass surface, which causes the nanodroplet to be stable on the glass surface.

On coated glass surfaces with polystyrene nanoparticles, due to the decrease in the surface energy and wettability, a transition from one to two separate clusters is observed, which is associated with the increase of surface coverage. It is observable that the rate of ballistic motion over the coated glass surfaces is lower than its motion on the bare surface due to decrease in the surface tension. On coated surfaces, water nanodroplets form and adsorb to the glass surface in the first two nano-seconds of simulation time. During the remainder of the simulation, the water nanodroplets shapes are stable on the substrate due to the formation of hydrogen bonding between water molecules and theirs pinning to the substrate. As seen in Fig. 4, the variation of second motions are increased associated with increasing the surface coverage,
implying a weakening of the nanodroplet pinning to the glass surface affiliated with the decrease of surface energy, which confirms transition of the surface wetting regime from hydrophilic to hydrophobic. It also shows that MSD is also directly related to the wettability and contact angle. The results show that the lower the MSD value, the bigger the contact angle. MSD and RMSD values for water molecules are in good agreement in the systems (Fig. 2-II and Fig. 4).

3.3. Contact angle estimation and modeling

For a solid substrate in contact with water molecules, wettability and contact angle results from a balance of cohesion and adhesion forces between water molecules and the surface, respectively [46]; therefore, there is a direct relation between surface energy and its contact angle. For same water droplet on different solid surfaces, higher surface energy
on the surface leads to lower contact angle. Based on this premise, contact angle is used as an indicator to investigate the effect polystyrene coating in various surface coverage percentage on the wettability of glass surface. The asymmetric distribution of surface energy on the glass surface leads to asymmetries in the nanodroplets, which are used in the calculations of the contact angle. These are noted more on bare glass surfaces due to overspreading, showing a variety in values in different directions. To minimize the effect of these variations in contact angle calculations (known as geometry effect), contact angles for each nanodroplet are calculated along the $z$-axis in the four main sides by image processing analysis, and then the mean of the measured values is considered as the nanodroplet contact angle (Fig. 5 and Table 2). The position of COMs for the water nanodroplets are also calculated along the $z$-axis (Fig. 6 and Table 2). As seen in Fig. 5 and Fig. 6, water molecules on the bare glass surface (GW) are highly spread, the contact angle is calculated to be about $25^\circ$, and the COM of nanodroplet is located in the distance of $4\,\text{Å}$ with respect to the glass surface. The calculated contact angle for water nanodroplets on the bare glass surface is in good agreement with experiments [47]. Penetration of water molecules into the glass surface grooves are also observed due to strong electrostatic interaction indicating Wenzel [48] state of wetting regime for bare glass surface.

Five percent covering of glass surface with polystyrene nanoparticle (GP05) leads the contact angle to increase from $25^\circ$ to $55.58^\circ$ and the position of COM of nanodroplet subsequently to shift to $11\,\text{Å}$ with respect to the glass surface. By increasing surface coverage percentage from five to ten (GP10), water molecules affinity with glass surface changes from hydrophilic to hydrophobic indicating 10% covering of glass surface with polystyrene nanoparticles is sufficient to create a favorable hydrophobic glass surface for flotation. Previously, Pelton et al. with lab-scale studies had shown that 10% covering of the glass surfaces with polystyrene nanoparticles could promote high flotation efficiencies by increasing the contact angle to more than $85^\circ$, whereas chemical collector requires at least 25% or higher coverage for a good recovery [11].

Compared to the one nanoparticle with 10% of surface coverage (GP10), using two nanoparticles with 5% of surface coverage for each one (G2P05) also causes the contact angle to increase to $93.07^\circ$ and the location of COM to shift to $15.4\,\text{Å}$ with respect to the surface. These results confirm that several smaller-sized nanoparticles compared to a larger-sized nanoparticle have a much better effect on reducing surface wettability. Lab-scale studies had shown that the use of polystyrene nanoparticles with the dimension of 46 nm compare to 120 nm produced far more satisfactory results in the glass flotation. The recovery of glass flotation with 10% covering of glass surface with 46 nm nanoparticles increased to more than 90% which confirms, the surface coverage with small size nanoparticle led to a more homogeneous and uniform coating of the surface and further reduced the adhesion forces between the glass surface and the water molecules [13].

On the relaxed glass surface (GsP10), 10% of surface coverage causes the contact angle to increase to $94.66^\circ$ and the location of COM for nanodroplet to shift to $15.5\,\text{Å}$ with respect to the glass surface showing fairly agreement with the energy analysis results. The process of stability for COMs is in good agreement with water RMSDs and MSDs (Fig. 2-II and Fig. 4 and Fig. 6). In general, the simulation results are in good agreement with experimental observations on real micro—macroscopic systems of various applications [11–14].

### 3.4. Water distribution

On a solid surface in immediate contact with water molecules, there is a direct relation between the arrangement of water molecules on the surface and surface energy [49,50]. Decreasing surface energy leads distances of water molecules from the surface to increase [51]. Density distribution profiles and distribution profiles of oxygen and hydrogen atoms in water molecules in the nanodroplets are used to investigate the positioning of water molecules on the glass surface as surface wettability indicator.

**Fig. 7** shows density distribution profiles of oxygen atoms in the water nanodroplets calculated along the $z$-axis as a function of distance

### Table 2

<table>
<thead>
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<th>GW</th>
<th>GP05</th>
<th>GP07</th>
<th>GP10</th>
<th>G2P05</th>
<th>GsP10</th>
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<td>11</td>
<td>12</td>
<td>15</td>
<td>15.4</td>
<td>15.5</td>
</tr>
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Fig. 6. Center of mass (COM) of water nanodroplets along $z$-axis with respect to glass surface.
from glass surface. In all density distribution profiles, two main peaks are observable, a major and minor, which show the location and thickness of interfacial and adjacent layers in the water nanodroplets with respect to the glass surface, respectively. In Fig. 7, GW shows the density distribution of the water nanodroplet on the bare glass surface. The major peak, which is located at the distance of 2.45 Å with respect to glass surface, represents strong non-bond interactions between water molecules and glass surface, wide spreading of water molecules on the glass surface, and dense accumulation of water molecules in the interfacial layer. In addition, the adjacent layer, minor peak, is located at the distance of 5.5 Å with respect to the glass surface.

On the coated glass surfaces with polystyrene nanoparticle, increasing the surface coverage percentage from five to ten leads the dense accumulation of water molecules in the interfacial layer to decrease. In addition, location of interfacial layer in the water nanodroplets shifts from 2.9 Å for GP05 to 3.41, 3.47, and 3.51 Å for GP10, G2P05, and GSp10, respectively. For coated glass surfaces with nanoparticles, the adjacent layers are also located at distances of 5.5 to 6 Å with respect to substrate. In addition, the convergence of water density to one (g·cm$^{-3}$) is observed at distances more than 8 Å with respect to the glass surface for all simulated nanodroplets. The results are generally in good agreement with previous reports [52].

For a target atom on a solid surface, distribution profile shows the number of atoms as a function of distance from the surface. Fig. 8 shows the distribution profiles of hydrogen and oxygen atoms in the nanodroplets along z-axis. On the bare glass surface (Fig. 8-GW), two successive peaks are observed, indicating the penetration zone and the interfacial layer, respectively. The first hydrogen and oxygen peaks with negative coordinate, which reveal the penetration of water molecules into glass surface grooves, confirm the dense accumulation of water molecules at the interfacial layer and the high possibility of forming hydrogen bonding between water molecules and glass surface. The first peaks also confirm Wenzel state of wetting regime for bare glass surface. The peaks coordinates confirm that oxygen atoms in water molecules present at the surface grooves are placed in lower levels compared to hydrogen atoms, which show water oxygen atoms in surface grooves arranged by the surface silicon atoms while water hydrogen atoms are located at the upper level. The second oxygen and hydrogen peaks show water molecules in the interfacial layer. The results also show that more than 30% of water molecules on the bare glass surface are present in immediate contact with the glass surface.

By increasing the percentage of surface coverage on the coated glass surfaces with polystyrene nanoparticles, as seen in Fig. 8, the effective non-bond interactions of glass surface interacting on water molecules decrease causing to gradual removal of the ordered water molecules on the glass surface grooves and change the shape of water nanodroplet on the surface to more spherical. In addition, the contact surface of water nanodroplets with substrate decreases, increasing the contact angle and the distance of COM from substrate surface. The gradual removal of water molecules on the surface grooves also indicates a gradual transition from a Wenzel state-wetting regime to a Cassie–Baxter state, associated with the increase of the surface coverage percentage with polystyrene nanoparticles.

### 3.5. Hydrogen bonding

The formation of hydrogen bonding between silicates and oxide minerals and water molecules is one of the most effective factors on strong wettability behavior of these minerals [53]; therefore, the number of hydrogen bonds per water molecule in nano-scale studies of silicates and oxide minerals can be used as a significant indicator of surface wettability [54]. To enhance surface hydrophobicity and minimize the possibility of forming hydrogen bonding between a silicate or oxide surface and water molecules, it is enough that water molecules to be located in a distance of more than 3 Å from the surface [55]. In flotation with common chemical collectors, this condition is achieved by coating a whole hydrophilic surface with a mono-layer of collector and reaching to critical micelle concentration (CMC) [56]. Nanoparticles as a collector have a different mechanism due to lack of complete surface coverage. By controlling and reducing a large amount of surface energy, the nanoparticles can minimize the tendency of uncoated sections of surface to adsorb water molecules and form hydrogen bonding.

As seen in Fig. 9, two kinds of hydrogen bonding are considered in these case studies to investigate the effect of polystyrene coating on glass surface wettability: (a) hydrogen bonding between water molecules and the glass surface, and (b) hydrogen bonds among water molecules. Fig. 10 and Fig. 11 show hydrogen-bonding structures in the simulated nanodroplets and the variation and the average number of
Fig. 8. Distribution profiles of hydrogen and oxygen atoms in water nanodroplets, (I): water molecules present at the glass surface grooves, (II): water molecules present at the interface.
hydrogen bonds per water molecule during last nano-second of simulation time, respectively. The distribution profile of the bare glass surface shows that more than 30% of water molecules in the interfacial layer of the nanodroplet are in immediate contact with glass surface. As seen in Fig. 10 and Fig. 11, this close positioning of water molecules leads a series of regular hydrogen bonds to form between water molecules and glass surface as well as pinning of the water nanodroplet to the surface. The average number of hydrogen bonds per water molecule is calculated to be around 3.8 hydrogen bonds which is in good agreement with previous studies [23]. In addition, the strong surface energy leads the arrangement of water molecules present in the interface layer to change to a tetrahedral molecular geometry.

Associated with the increase of surface coverage percentage with polystyrene nanoparticles, a decrease in the average number of hydrogen bonds per water molecules is observed. In the GP05 system, 5% of surface coverage reduces the surface energy causing water molecules to increase the separation distance from the surface. Accordingly, the average number of hydrogen bonds per water molecule reduces to about 3.6. As seen in Fig. 10, regular hydrogen bonds between water molecules and the glass surface also show a decreasing trend in the simulation systems.

By increasing surface coverage percentage to ten (GP10, G2P05, and GsP10), the average number of hydrogen bonds per water molecule gradually converges to flickering clusters [57,58], with the hydrogen bond numbers typical of bulk water molecules. For these cases, the hydrogen bond numbers are calculated to be between 3.2 and 3.4 bonds per water molecule confirming the low affinity of water molecules to the glass surface. The minimum number of hydrogen bonds per water molecule is encountered for the system GsP10 due to silicon termination of the relaxed form of glass surface, which is reasonable.

4. Concluding remarks

Molecular dynamics is used to perform a feasibility study on using hydrophobic nanoparticle as a collector in flotation. Glass and stabilized hydrophobic polystyrene in various sizes are chosen as substrate and nanoparticle, respectively. To evaluate the wettability behavior of the glass surface, qualitative energy analyses are performed on both

Fig. 9. (I) Hydrogen bonds between hydrogen atoms in water molecules and oxygen atoms in glass surface, (II) hydrogen bonds among water molecules.
unrelaxed and relaxed forms of the glass surface. Despite significant difference in values, surface energies on both surface forms show a heavy asymmetric distribution, making the glass surface strongly hydrophilic. However, the covering of glass surface with polystyrene nanoparticles reduces surface tension and changes the wettability behavior of the glass surface from hydrophilic to hydrophobic. Unlike classical chemical collectors, a partial coating of glass surface with polystyrene nanoparticles, up to 10%, leads to major changes in glass surface wettability. In addition, associated with this coverage, we observe a transition from one to two separate clusters in water molecules adsorption on the surface and a gradual transition of the surface-wetting regime from the Wenzel to Cassie–Baxter state. The average number of hydrogen bonds per water molecule converges to the values typical of bulk water. The results also confirm that at the same surface coverage, the smaller the nanoparticles, the higher the hydrophobicity of the surface. In general, the results are in good agreement with previous lab-scale studies and show that nanoparticles can be considered as one of the promising alternatives for new types of flotation reagents.

Acknowledgments

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.molliq.2018.11.062.
Fig. 11. Number of hydrogen bonds per water molecules calculated as a function of time during last nanosecond of simulation.

References


