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Adsorption Mechanism of Linear Alkane Liquid in Contact with Face Centred Cubic Lattice

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ABSTRACT

Adsorption mechanisms is related to wear rates and scar. The main contributor of these problems is adsorption of liquid on solid surfaces. However, these problems have yet to be explained in the aspect of liquid orientation. Thus, this study investigates the adsorption mechanisms of butane and pentane in contact with face- centred cubic (FCC) lattice of (110), (100) and (111) surfaces, using molecular dynamics simulations. A constant temperature system will be applied to the system and the adsorption mechanism is explained using structural quantities. The results show similar trends where a large adsorption of liquid appears on the solid surfaces and the liquid orientation is in parallel with the solid surfaces. However, the differences appear in the peak height of the adsorption of liquid for the systems. It is found that, (111) exhibits the highest adsorption of liquid near the solid liquid interfaces. Whereas, in terms of elongation of liquid alkanes (110) surface shows large elongation value in the x-directions. From these findings, it suggests that the alkane liquid is adsorbed on the solid surfaces that decreases with the increase in liquid molecule length. Furthermore, the surface structure of the solid influences the orientation of liquid on the solid surface.

1. Introduction

Solid in contact with liquid also known as solid-liquid (S-L) interfaces is commonly found in many engineering applications such as thermal interface material [1], lubrication and coating [2], cooling of electronic equipment [3] and many more. In the study of nanoscale materials understanding the equilibrium and non-equilibrium properties at the vicinity of S-L interfaces is crucial. When the thickness of the interfaces is in nanometre the macroscopic theory and physics are anomalous ant not easily determined, since the interaction is governed by molecular interaction between solid and liquid molecules [4,5]. Thus, in order to reproduce and replicate the liquid behaviour in the nanoscale,

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Molecular dynamics (MD) simulation is suitable tools with confirm studies with reliable inter and intra molecular interaction models [6,7].

In the thermal transport across Solid-liquid (S-L) interfaces of liquid films, there exists a phenomenon of temperature discontinuity between the solid walls and the liquid films. In the context of molecular dynamics (MD), the temperature discontinuity at these interfaces is affected by the interactions between solid and liquid molecules [8,9], as well as the roughness of the solid walls in contact with the liquid film [10,11]. Khare *et al.,* [8,9] investigated the transfer of thermal energy and momentum at the S-L interface, comparing the thermal boundary resistance (TBR) between shear and non-shear systems. Their study utilized model liquid molecules that were characterized by strong and weak interaction forces with the solid atoms, specifically in contact with the (100) crystal plane of the solid walls. Previous research has predominantly relied on simplified liquid models that do not account for bond bending and torsional motions when examining thermal energy transfer at the interfaces [8-11]. As a result, the influence of crystal planes on actual liquids of varying molecular lengths and the effect of molecular liquid with branches remains inadequately understood.

In further reading it is understood that, the knowledge of transport properties at the solid-liquid interface plays a significant role in the understanding of liquid adhesion [12,13], liquid diffusion [14,15] and wettability [16,17] which can be summarized as adsorption mechanism. In the past the performance of lubrication is determine by adsorption of liquid lubricant on solid surfaces [18,19] and surface morphology of the solid surfaces [20,21], however the clear explanation of the liquid on the solid surfaces in molecular level have yet to be explained. Thus, this paper is interested to investigate the adsorption mechanism of linear alkane liquid on solid surfaces with basic surface structure of face-centred cubic (FCC) lattice of (100), (110) and (111) planes using non-equilibrium molecular dynamics (NEMD) simulations. In this study the structural quantities which are the density distributions, radius of gyration and orientation order parameter will be evaluated to explain the adsorption mechanisms.

2. Methodology

2.1 Simulation Model

Solid-liquid interfaces system of these study is modelled by liquid placed in between two layers of solid as shown in Figure 1. The layers between solid and liquid are referred to as solid-liquid (S-L) interfaces in this investigation. In this investigation liquid alkanes namely butane and pentane have been utilized. As for the solid surface, the face-centred cubic (FCC) lattice has been utilized. In most engineering surfaces consisted of the crystal structure. FCC surfaces are the very basic structure and have been widely used in past studies to clarify surface characteristics [4,22,23]. There were three types of surfaces in FCC namely are (100), (110) and (111) planes that are in contact with the liquid alkanes. In all the simulation system only one type of FCC surface is utilized on the left and right sides of the simulation system and one type of liquid alkane is utilized for one simulation.

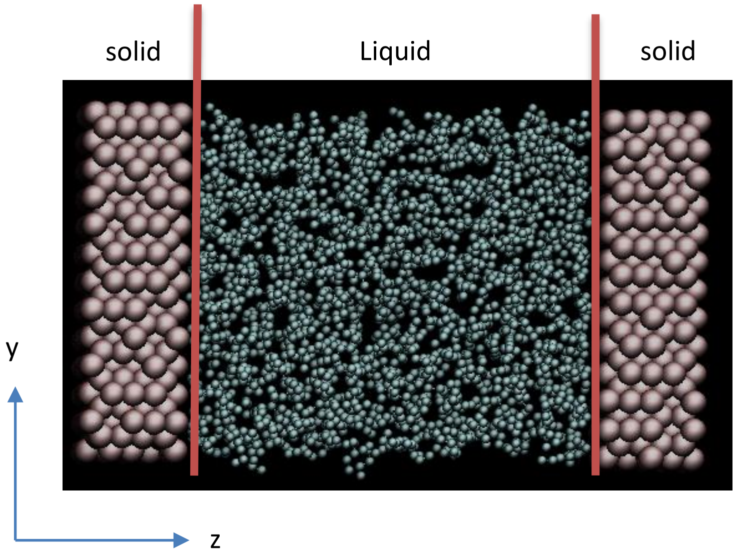

Fig. 1. A snapshot of liquid butane in between layers of solid

2.2 Periodic Boundary Condition and Simulation Size

In this simulation, to make sure that the alkane liquid behaves like the actual liquid. The system is modelled in such a way that the attraction and repulsion forces from the layers solid do not influence the centre of the liquid. Furthermore, to replicate the system as the actual conditions, the layers of solid on both sides of the simulation system were set to be fixed in the z-direction. This condition replicates the condition of extremely large surface in contact with liquid film. Thus, the periodic boundary condition of this simulation system is only set on the x and y-axes. Although there are slight variations in the volume of the simulations systems.

2.3 Attraction and Repulsion Forces

In Molecular dynamics simulations, in order to model the liquid's attraction and repulsion forces. It was replicated by potential functions. For the liquid, there are several types of potential forces available namely are Anistropic united atom model [24], All atom model [25] and united atom model [26]. In this simulation the united atom has been utilized due to the computation time and accuracy of the results. Thus, in this paper united atom NERD potential has been utilized. The same kind of interaction forces have been utilized in past investigation in refs [4,23,27]. In the United atom NERD potentials, the CH3 and CH2 atom is grouped in a single interaction sites represented as pseudo atom. The pseudo atom connected to each other forming a long chain molecule of butane and pentane. NERD potentials consisted of three types of bonded interaction forces and one type of non-bonded interaction forces. The three types of interaction forces are bond bending, bond stretching and torsion. Whereas the non-bonded interaction forces are the van der Waals interactions. The bond bending interaction in the interaction that takes place forces are as follows:

$$U(\theta) = \frac{k_\theta}{2}(\theta - \theta_o)^2 \tag{1}$$

Where $k_\vartheta = 8.6291 \times 10^{-19}$ j/rad^2 and $\theta_0 = 114.0°$. The bond stretching is the interaction between two pseudo atom which are given as follow:

$$U(r_{ij}) = \frac{k_r}{2}(r_{ij} - b_{eq})^2 \quad (2)$$

Where k_r =1.3323 × 10^{-18} and b_{eq} = 1.54 Å. For the torsion interaction, it is defined as the interaction between any four neighbouring pseudo atoms. The interaction forces are given as follows:

$$U(\varphi) = V_o + V_1(1 + cos\,\varphi) + V_2(1 - cos\,2\,\varphi) + V_3(1 + cos\,3\,\varphi) \quad (3)$$

Where V0 = 0 J, V1 = 4.9018 × 10^{-21} J, V2 = −9.4146×10^{-22} J and V3 = 1.0925×10^{-20} J [4,5].

For the solid numerous types of Morse potential is utilized which is the similar potential that has been used for past investigations [4,23,27]. The equation is given as follows:

$$\Phi(r_{ij}) = D[e^{-2\alpha(r_{ij}-r_o)} - 2e^{-\alpha(r_{ij}-r_o)}] \quad (4)$$

where D is 7.6148 × 10^{-13} erg, r_0 is 3.0242 Å and α is 1.5830 Å^{-1} [4,23,27]. The interaction forces between intra-molecular interaction are Universal Force Fields (UFF). The UFF potential forces are given as follows:

$$U^{LJ}(r_{ij}) = 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right] \quad (5)$$

Where r_{ij} is the distance between pseudo-atom *i* and *j*. The interaction parameter was calculated using Lorent-Bertholet (LB) combining rules [19,23]. which are given as follow:

$$\varepsilon_{ij} = \sqrt{\varepsilon_{ii}\varepsilon_{jj}} \quad (6)$$

and

$$\sigma_{ij} = \frac{\sigma_{ii}+\sigma_{jj}}{2} \quad (7)$$

The same kind of interaction forces have been utilized in a number of past investigations given in references [4,5,19,23].

2.4 Details of Simulation step

In general, molecular dynamics simulation comes from resultant forces that act on a molecule. The resultant force predicted the movement of the molecule in each step. However, for the cases of many molecules present in a simulation model, the prediction of the molecule movement is replaced by algorithm. In this simulation, reversible reference propagator algorithm with multiple time step is utilized that calculates the forces via intermolecular motion and intramolecular motion in 1 femto second and 0.2 femto second, respectively.

The temperature of the simulation was first raised slowly to the targeted temperature for 1-to-2-million-time step. In these simulations the targeted temperature is 0.7 of the critical temperature of the liquid. After the simulation system reaches the targeted temperature, it is maintained at the targeted temperature until a uniform temperature is achieved throughout the simulation system for

3 to 4 million time-steps. Once the uniform temperature is achieved, the data acquisition step takes place where 4 to5 million time-steps are run at the uniform temperature of the simulation system.

3. Results and Discussions

3.1 Density Profiles

Density profile play a significant role in molecular dynamics simulation. It gives an insight of the liquid behaviour in the solid and liquid interfaces system and also have been utilized as a validation simulation model. In this study the simulation model has been validated using the density profile of butane [27] and pentane [28].

Figure 2 and Figure 3 show the density profile of simulation model of layers of solid with FCC (100) contacting liquid pentane and butane, respectively. The blue line is the density profiles of the liquid and the orange line the density profiles of the solid. Since, almost similar profiles is observed for other types of crystal planes regardless the types of liquid, only the liquid in contact with FCC (100) is shown here. As observed in both figures, the density profiles for the liquid creates a number of peak and valleys near the solid surfaces that decreases as the distance move towards the centre of the simulation systems. A flat line appears at the centre of the simulation systems, approximately at the 520 kg/m^3 for butane and 570 kg/m^3 for pentane. These are the values of density for butane and pentane at the 0.7 of the critical temperature. Since the flat line appears approximately at the said value, it is representing that the liquid in this simulation system are exactly in the liquid form.

The peaks and valleys appear near the solid and liquid interfaces can be referred to as adsorption layers after this. These adsorption layers are created from the attraction forces and repulsion forces coming from the solid surfaces. And at the centre of the simulation system the flat line shows that there are no significant attraction forces and repulsion forces affected the liquid. Based on the observation, it is found that the adsorption layers next to solid layers shows the highest value and slowly diminishes as it goes to the centre of the simulation system. The highest adsorption layer shows that a large number of liquid molecules are attracted to the solid surface that creates a solid like layer next to the actual solid layers.

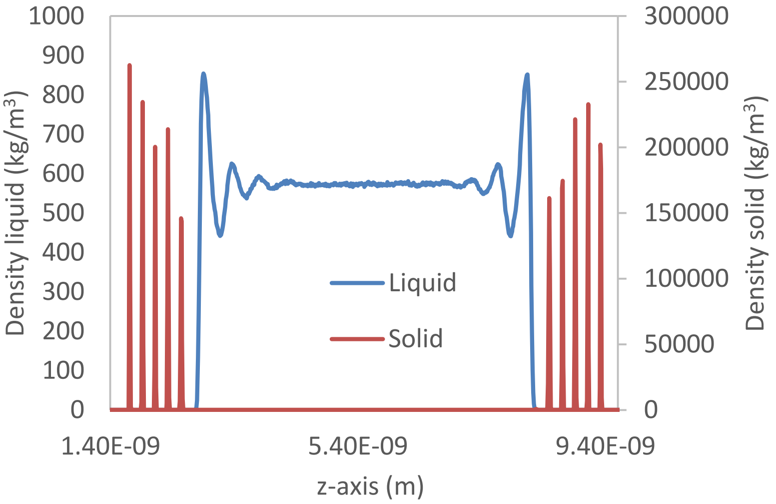

Fig. 2. Density profile of liquid pentane in between two layers of solid with FCC (100) surfaces

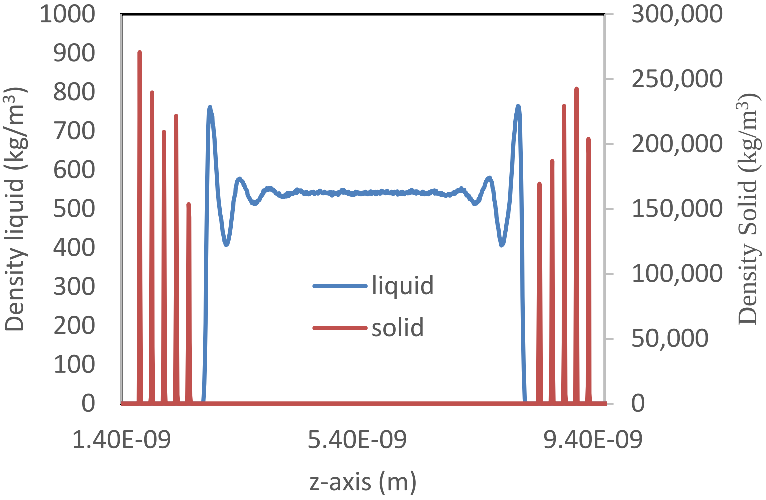

Fig. 3. Density profile of liquid butane in between two layers of solid with FCC (100) surfaces

Figure 4 shows the super imposed position of density profiles for FCC (100), (110) and (111) contacting liquid butane. Since, almost similar profiles is observed only density profiles of liquid butane is shown here. In addition, on the left sides of the density profiles is shown here due to the profiles is approximately symmetry as observed in the figure, the adsorption layer closest to the solid has the highest peak values compared to the rest. Furthermore, there exists slight variation in the height of the adsorption layers, it is found that FCC(111) has the highest value of peak height follow by FCC(100) and FCC(110). This value has been predicted since, the number of solid molecules appear near the interfaces of solid and liquid is the highest for FCC (111). Thus, based on the figure it can be concluded that the solid like layers of the adsorption layer appear due to the forces coming from solid surfaces and the height of the adsorption layer depend closely on the number of solid molecules appear near the interfaces of solid and liquid.

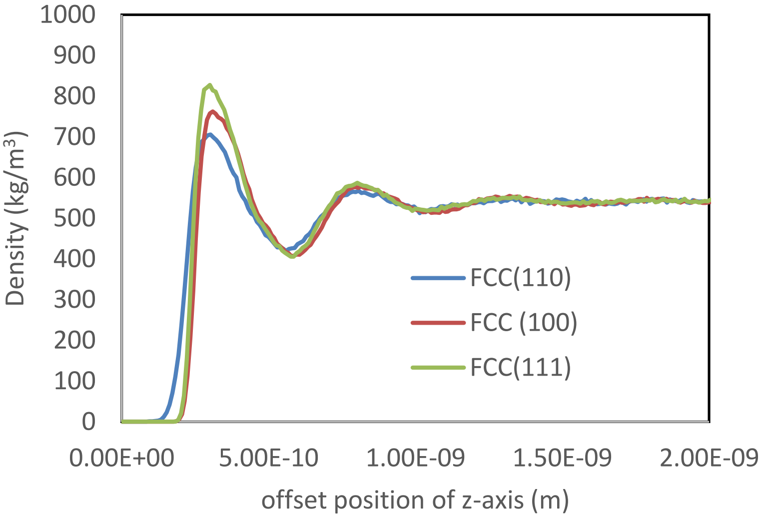

Fig. 4. Density profiles of FCC (100), (110) and (111) contacting liquid butane using offset position of z-axis

3.2 Radius of Gyration

In order to further clarify the characteristics of the liquid adsorption behaviour near the interfaces of solid-liquid, the radius of gyration is calculated for each of the simulation model. Radius gyration is a method used to identify the shape of molecules for liquid in a liquid film. In this investigation the radius gyration is calculated based on the average distance of each atom presence in the molecule o the centre of the molecules.

Figure 5 shows the radius of gyration of liquid pentane and butane contacting FCC (100) surface. As observed in the figure on average, radius of gyration for pentane is higher than butane. And regardless of the types of liquid the value of the radius of gyration is higher at the solid surfaces and start to shows average value at the centre of the simulation systems. Since the same kind of profile have been observed on the left and right sides of the simulation system only the left sides is shown in the figure.

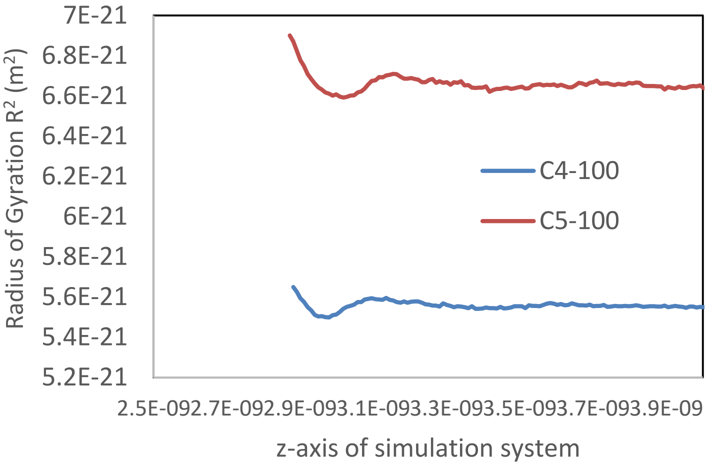

Fig. 5. Radius of gyration for pentane and butane facing FCC (100)

Figure 6 shows the radius of gyration for liquid pentane in contact with FCC (100), (110) and (111). Only the figure of radius of gyration for liquid pentane is shown in the figure since both liquids shows approximately similar characters. Based on the figure the value of radius gyration shows the highest near the solid surfaces. Among the three types of crystal plane, FCC (110) shows the highest value followed by FCC (111) and last is FCC (100). Although in the density profiles FCC (110) shows the lowest peak height however in the radius of gyration the values is the highest.

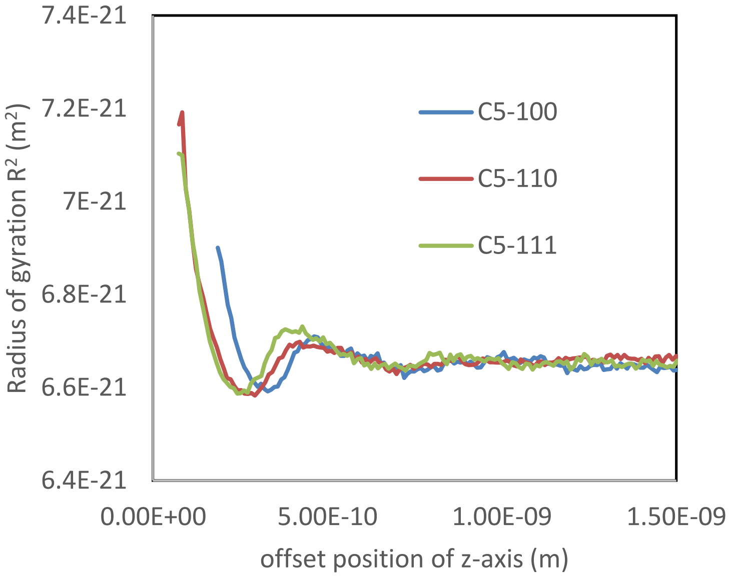

Fig. 6. Radius of gyration for pentane facing FCC (100), (110) and (111)

In order to further identify the shape of the liquid in the liquid film, the radius of gyration is further decomposed into x, y and z-axes. Figure 7, Figure 8 and Figure 9 shows the radius of gyration for FCC (110), (100) and (111) in the x-, y- and z-axes. It is found that, for the case of x- and y-axes, the radius gyration shows a high value near the solid surfaces and a flat line is observed at the centre of the simulation systems. The same kind of behaviour have been observed in all FCC surfaces and regardless the type of liquid. Based on close observation it is found that the radius of gyration value for FCC (111) is slightly higher than FCC (100). This kind of behaviour is predicted due to the large adsorption layers of density profile is also observed for density profile of FCC(111). However, an extremely large value is observed for liquid pentane in contact with FCC (110) as shown in Figure 8. A larger value of x-axis is found here. This is due to the surfaces structure of the solid surfaces. As we all know, that the molecules arrangement for FCC (110) has a larger peak and valleys in the x-directions. And based on the results of radius of gyration decomposed into x-, y- and z-axes shows that the shape for FCC(110) is the highest which predict that the liquid is trapped inside the valleys of the surface structure of FCC (110). Since the same kind of characteristics is observed liquid butane only liquid pentane results are shown here. In addition, although the characteristics is almost similar however on average, the value of radius of gyration for liquid pentane is slightly higher than liquid butane.

3.3 Significant of the Results to the Potential Applications

In overall the findings of the results shows that liquid of alkane is normally adsorbed on solid surfaces and the liquid are oriented in parallel with solid surfaces regardless the surface structure. This kind of liquid adsorption mechanism shows close relation with wear rates and scar. The wear rates of contact surfaces are coming from the lack of liquid adsorption on solid surfaces thus producing large scar at the contact interfaces [2]. Based on these results, the identification of liquid with high adsorption on solid surfaces is crucial in order to overcome or reduce the implication of wear rates and scar that happen at the contact interfaces. On the other hand, in the case of electronic cooling, there exists thermal paste that have been applied at the contact interfaces between computer processor and heat sink . This kind of applications look at the heat transfer at the contact of thermal paste (can be consider as liquid) and solid of the heat sink [3].

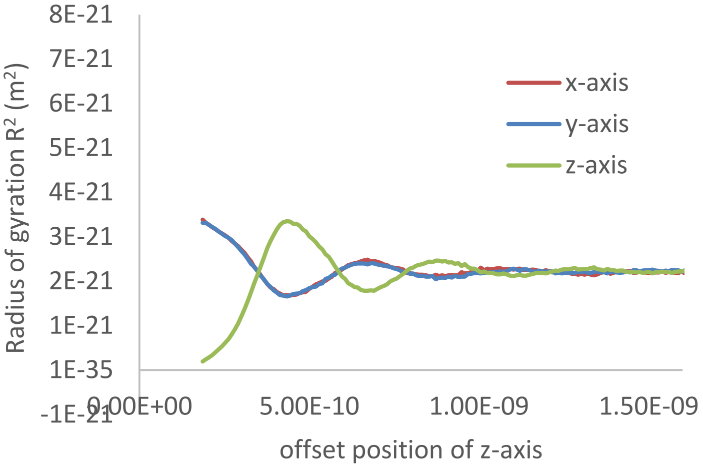

Fig. 7. Radius of gyration decomposed into x-, y- and z-axes for pentane liquid contacting FCC (100)

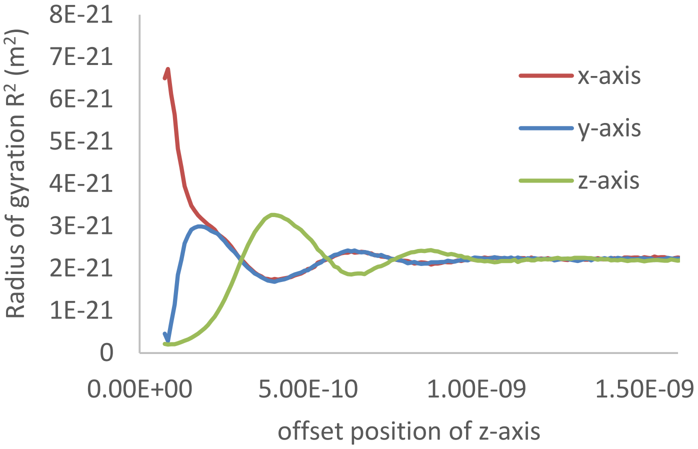

Fig. 8. Radius of gyration decomposed into x-, y- and z-axes for pentane liquid contacting FCC (110)

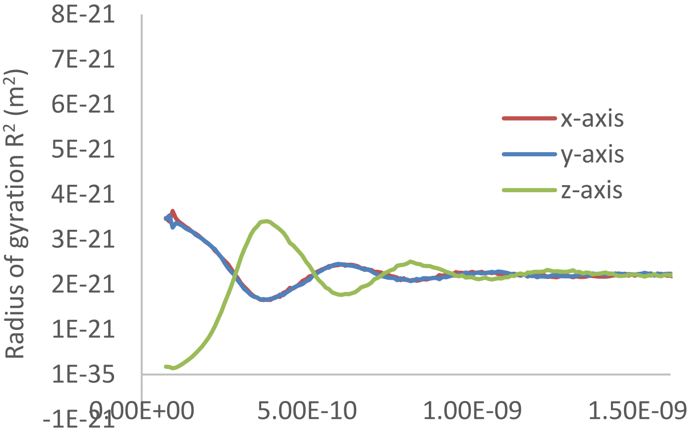

Fig. 9. Radius of gyration decomposed into x-, y- and z-axes for pentane liquid contacting FCC (111)

4. Conclusions

In this study the, adsorption mechanism of linear alkane liquid is investigated using molecular dynamics simulation at a constant temperature. The adsorption mechanism of the linear alkane liquid was explain based on the density profiles and radius of gyration for the liquid. Based on the findings, it is concluded that, the behaviour of liquid adsorption on solid surface depends closely on the number of solid molecules present near the interfaces of solid liquid. In addition, the adsorption mechanism is also affected by the characteristics of the surface structure for solid. According to the current results the effect of surface structure has a higher effect toward the liquid orientation on the solid surfaces.

The results are significant to the specific studies of journal bearing application and thermal interface materials. However further investigation in term of different types of materials and lubrication or liquid is crucial and should be explored in the future. Based on past studies of non-equilibrium molecular dynamics simulation (NEMD) it is found that, the combination of solid and liquid play a significant role in the adsorption mechanism and heat transport at the interfaces [4,5,19,23]. To the best of the authors knowledge these problems have not been explored yet. Thus, future investigation should be focusing more on different types of liquid and surfaces.

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References

[1] Guo, Xiaoxiao, Shujian Cheng, Weiwei Cai, Yufeng Zhang and Xue-ao Zhang. "A review of carbon-based thermal interface materials: Mechanism, thermal measurements and thermal properties." *Materials & Design* 209 (2021): 109936. https://doi.org/10.1016/j.matdes.2021.109936

[2] Liu, Heli, Huaiju Liu, Caichao Zhu and Robert G. Parker. "Effects of lubrication on gear performance: A review." *Mechanism and Machine Theory* 145 (2020): 103701. https://doi.org/10.1016/j.mechmachtheory.2019.103701

[3] Dinh, Toan, Hoang-Phuong Phan, Navid Kashaninejad, Tuan-Khoa Nguyen, Dzung Viet Dao and Nam-Trung Nguyen. "An on-chip SiC MEMS device with integrated heating, sensing and microfluidic cooling systems." *Advanced materials interfaces* 5, no. 20 (2018): 1800764. https://doi.org/10.1002/admi.201800764

[4] Saleman, Abdul Rafeq bin, Hari Krishna Chilukoti, Gota Kikugawa and Taku Ohara. "A molecular dynamics study on the thermal rectification effect at the solid–liquid interfaces between the face-centred cubic (FCC) of gold (Au) with the surfaces of (100),(110) and (111) crystal planes facing the liquid methane (CH4)." *Molecular Simulation* 45, no. 1 (2019): 68-79. https://doi.org/10.1080/08927022.2018.1535177

[5] Liu, Xiao, Donatas Surblys, Yoshiaki Kawagoe, Abdul Rafeq Bin Saleman, Hiroki Matsubara, Gota Kikugawa and Taku Ohara. "A molecular dynamics study of thermal boundary resistance over solid interfaces with an extremely thin liquid film." *International Journal of Heat and Mass Transfer* 147 (2020): 118949. https://doi.org/10.1016/j.ijheatmasstransfer.2019.118949

[6] Saleman, Abdul Rafeq bin, Hari Krishna Chilukoti, Gota Kikugawa and Taku Ohara. "A molecular dynamics study on the thermal rectification effect at the solid–liquid interfaces between the face-centred cubic (FCC) of gold (Au) with the surfaces of (100),(110) and (111) crystal planes facing the liquid methane (CH4)." *Molecular Simulation* 45, no. 1 (2019): 68-79. https://doi.org/10.1080/08927022.2018.1535177

[7] Matsubara, Hiroki, Gota Kikugawa, Takeshi Bessho, Seiji Yamashita and Taku Ohara. "Molecular dynamics study on the role of hydroxyl groups in heat conduction in liquid alcohols." *International Journal of Heat and Mass Transfer* 108 (2017): 749-759. https://doi.org/10.1016/j.ijheatmasstransfer.2016.12.045

[8] Khare, Rajesh, Pawel Keblinski and Arun Yethiraj. "Molecular dynamics simulations of heat and momentum transfer at a solid–fluid interface: relationship between thermal and velocity slip." *International journal of heat and mass transfer* 49, no. 19-20 (2006): 3401-3407. https://doi.org/10.1016/j.ijheatmasstransfer.2006.03.005

[9] Khare, Rajesh, Juan de Pablo and Arun Yethiraj. "Molecular simulation and continuum mechanics investigation of viscoelastic properties of fluids confined to molecularly thin films." *The Journal of Chemical Physics* 114, no. 17 (2001): 7593-7601. https://doi.org/10.1063/1.1361077

[10] Barisik, Murat and Ali Beskok. "Temperature dependence of thermal resistance at the water/silicon interface." *International Journal of Thermal Sciences* 77 (2014): 47-54. https://doi.org/10.1016/j.ijthermalsci.2013.10.012

[11] Barisik, Murat and Ali Beskok. "Temperature dependence of thermal resistance at the water/silicon interface." *International Journal of Thermal Sciences* 77 (2014): 47e54. https://doi.org/10.1016/j.ijthermalsci.2013.10.012

[12] Fadzullah, SH Sheikh Md, M. M. Nasaruddin, Z. Mustafa, W. A. W. A. Rahman, G. Omar, M. A. Salim and M. R. Mansor. "The effect of chemical surface treatment on mechanical performance of electrically conductive adhesives." (2020): 444-451. https://doi.org/10.5109/4068625

[13] Merabia, Samy, Julien Lombard and Ali Alkurdi. "Importance of viscoelastic and interface bonding effects in the thermal boundary conductance of solid–water interfaces." *International Journal of Heat and Mass Transfer* 100 (2016): 287-294. https://doi.org/10.1016/j.ijheatmasstransfer.2016.04.043

[14] Chilukoti, Hari Krishna, Gota Kikugawa, Masahiko Shibahara and Taku Ohara. "Local thermal transport of liquid alkanes in the vicinity of α-quartz solid surfaces and thermal resistance over the interfaces: A molecular dynamics study." *Physical Review E* 91, no. 5 (2015): 052404. https://doi.org/10.1103/PhysRevE.91.052404

[15] Saleman, Abdul Rafeq, Fudhail Abdul Munir, Mohd Rody Mohammad Zin, Mohd Shukri Yob, Gota Kikugawa and Taku Ohara. "Heat transport at solid-liquid interfaces between face-centered cubic lattice and liquid alkanes." *Journal of Advanced Research in Fluid Mechanics and Thermal Sciences* 44, no. 1 (2018): 123-130.

[16] Wang, Zhangxin, Menachem Elimelech and Shihong Lin. "Environmental applications of interfacial materials with special wettability." *Environmental science & technology* 50, no. 5 (2016): 2132-2150. https://doi.org/10.1021/acs.est.5b04351

[17] Ramos-Alvarado, Bladimir, Satish Kumar and G. P. Peterson. "On the wettability transparency of graphene-coated silicon surfaces." *The Journal of chemical physics* 144, no. 1 (2016). https://doi.org/10.1063/1.4938499

[18] Zhang, Shaohua, Yijun Qiao, Yuhong Liu, Liran Ma and Jianbin Luo. "Molecular behaviors in thin film lubrication—Part one: Film formation for different polarities of molecules." *Friction* 7 (2019): 372-387. https://doi.org/10.1007/s40544-019-0287-1

[19] Podgornik, B., M. Sedlaček and Dj Mandrino. "Performance of CrN coatings under boundary lubrication." *Tribology international* 96 (2016): 247-257. https://doi.org/10.1016/j.triboint.2015.12.039

[20] Sundararajan, G., S. V. Joshi and L. Rama Krishna. "Engineered surfaces for automotive engine and power train components." *Current opinion in chemical engineering* 11 (2016): 1-6. https://doi.org/10.1016/j.coche.2015.10.001

[21] Chung, Pil Seung, Myung S. Jhon and Hyoung Jin Choi. "Molecularly thin fluoro-polymeric nanolubricant films: tribology, rheology, morphology and applications." *Soft matter* 12, no. 11 (2016): 2816-2825. https://doi.org/10.1039/C5SM02434J

[22] Kikugawa, Gota, Taku Ohara, Tohru Kawaguchi, Ikuya Kinefuchi and Yoichiro Matsumoto. "A molecular dynamics study on heat conduction characteristics inside the alkanethiolate SAM and alkane liquid." *International Journal of Heat and Mass Transfer* 78 (2014): 630-635. https://doi.org/10.1016/j.ijheatmasstransfer.2014.07.040

[23] Kikugawa, Gota, Taku Ohara, Toru Kawaguchi, Eiichi Torigoe, Yasumasa Hagiwara and Yoichiro Matsumoto. "A molecular dynamics study on heat transfer characteristics at the interfaces of alkanethiolate self-assembled monolayer and organic solvent." *The Journal of chemical physics* 130, no. 7 (2009). https://doi.org/10.1063/1.3077315

[24] Nieto-Draghi, Carlos, Philippe Ungerer and Bernard Rousseau. "Optimization of the anisotropic united atoms intermolecular potential for n-alkanes: Improvement of transport properties." *The Journal of chemical physics* 125, no. 4 (2006). https://doi.org/10.1063/1.2219114

[25] Siu, Shirley WI, Kristyna Pluhackova and Rainer A. Böckmann. "Optimization of the OPLS-AA force field for long hydrocarbons." *Journal of Chemical theory and Computation* 8, no. 4 (2012): 1459-1470. https://doi.org/10.1021/ct200908r

[26] Müller, Erich A. and Andres Mejia. "Comparison of united-atom potentials for the simulation of vapor–liquid equilibria and interfacial properties of long-chain n-alkanes up to n-c100." *The Journal of Physical Chemistry B* 115, no. 44 (2011): 12822-12834. https://doi.org/10.1021/jp203236q

[27] Bin Saleman, Abdul Rafeq, Hari Krishna Chilukoti, Gota Kikugawa, Masahiko Shibahara and Taku Ohara. "A molecular dynamics study on the thermal transport properties and the structure of the solid–liquid interfaces between face centered cubic (FCC) crystal planes of gold in contact with linear alkane liquids." *International Journal of Heat and Mass Transfer* 105 (2017): 168-179. https://doi.org/10.1016/j.ijheatmasstransfer.2016.09.069

[28] Nhung, Nguyen Thi Ai and Pham Van Tat. "Diagram of vapor-liquid equilibria for n-pentane using hybrid Gibbs ensemble Monte Carlo simulation." *Vietnam Journal of Chemistry* 58, no. 1 (2020): 101-107. https://doi.org/10.1002/vjch.2019000148