SEMARAK ILMU PUBLISHING

Journal of Advanced Research in Applied Mechanics

Journal homepage:
https://semarakilmu.com.my/journals/index.php/appl_mech/index
ISSN: 2289-7895

Investigating Roughness Effect to Geometrically Necessary Dislocation in Micro-Indentation using Finite Element Analysis

Weng Mei Kok[1], Heoy Geok How[1,*], Hun Guan Chuah[1], Yew Heng Teoh[2]

[1] Department of Engineering, UOW Malaysia KDU Penang University College, 10400 Georgetown, Malaysia
[2] School of Mechanical Engineering, Engineering Campus, Universiti Sains Malaysia, Seri Ampangan, Nibong Tebal, Pulau Pinang, 14300, Malaysia

ARTICLE INFO

Article history:
Received 29 December 2022
Received in revised form 23 February 2023
Accepted 3 March 2023
Available online 23 March 2023

Keywords:
Geometrically necessary dislocation; surface roughness; hardness; size effect; Finite Element Analysis

ABSTRACT

Surface roughness is a well-known factor in effecting to the hardness value in low indentation depth. The rougher surface induces a greater hardness value. However, the hardening mechanisms, such as the effect of geometrically necessary dislocations (GNDs), with surface roughness is rarely discussed. Therefore, the current study revealed the relationship between the surface roughness effect and the material dislocation through GNDs by using finite element analysis. 3D Crystal plasticity finite element indentation model was developed with various surface roughness between 24 to 140 nm and a range of indentation depth 3.55 to 12.27 µm to indent on the copper (111) material. The experimental indentation work was performed to validate the finite element model. The surface roughness was discovered to contribute to GND density. The GNDs distribution is highly dependent on the geometry of surface asperities, as the surface get rougher the GNDs distribution tends to be inhomogeneous. The GND density is exponentially proportional to the roughness effect. The GND density increases from 3.58×10^{14} m^{-2} for surface roughness 24 nm to 1.01×10^{15} m^{-2} for surface roughness 140 nm at indentation depth 3.55 µm. Therefore, GND density which contributes to hardening effect causes rougher surface to induce greater hardness value.

1. Introduction

Indentation is commonly used to measure the material properties such as hardness and Young's modulus of the material. The indenter moves towards the material and leaves an imprint when the indenter is removed. In macro-indentation, the hardness is found to be constant with load. In the latter, the hardness was found to vary in micro- and nano- scale. The hardness decreases as the indentation load increases which is known as indentation size effect (ISE). Many factors, including surface roughness, indenter tip radius, oxidation, and crack formation, contribute to ISE. McElhaney *et al.,* [1] found the hardness of polycrystalline copper and single copper (111) increase at small indentation depth. Nix and Gao [2] described the ISE with the concept of Geometrically Necessary Dislocation (GND) and they showed the relation perfectly fitted McElhaney *et al.,* hardness data. GND

* *Corresponding author.*
E-mail address: heoygeok.how@uow.edu.my

https://doi.org/10.37934/aram.104.1.2532

density is a type of dislocation mechanism that contributes to the hardening effect. This mechanism involves either storing the dislocations for compatible deformation or accumulating and trapping them into each other, which restricts the dislocation motion. Huang *et al.,* [3] fitted with Nix-Gao model which the hardness value increased as the indentation depth decreased. However, previous studies did not quantify the surface roughness before investigating their studies, leading to a deviation in result when replicating previous study.

Surface roughness is a well-known factor in contributing to the ISE. Numerous studies revealed surface roughness is sensitive to the hardness value. Chen *et al.,* [4] investigated the Young's modulus and hardness of AISI 316L stainless steel increased on rougher surface using finite element simulation. The rougher surface was found to exhibit a more pronounced asymmetrical strain distribution. Chuah and Ripin [5] developed a roughness dependent friction model using finite element method. The model was fitted to the experimental results and a greater frictional effect was found on the rougher surface. Most of the experimental results found that the rougher surface produced a greater hardness value, while Jiang *et al.,* [6] and Kim *et al.,* [7] obtained an opposite trend, where the smoother surface produced a greater hardness value. To address the opposite trend between surface roughness and hardness value, Tang *et al.,* [8] simulated the effect of different positions of the indenter tip on the surface. The position of the indenter tip on the valley and peak of the surface asperities generated a higher and lower hardness value, respectively, when compared to the perfectly flat surface. They suggested that the opposite trend of surface roughness and hardness value was caused by the large amplitude-to-wavelength ratio of the surface asperities, which led to the presence of a side bending effect.

Although the relationship between surface roughness and hardness was found during indentation, no further investigation has been conducted on the dislocation mechanism, such as GND density response to the effect of surface roughness. Javid *et al.,* [9] and Qu *et al.,* [10] found out the GND density increased as the indentation depth decreased for tungsten and copper material, respectively. The increase in hardness value at smaller indentation depths was due to the presence of high GND density. However, Demir *et al.,* [11] revealed the GND density increased with indentation depth for copper material, which contradicted the Nix-Gao model. Their findings revealed that the distribution of GND density was observed to be inhomogeneous across all indentation depths. They suggested the opposite conclusion was applicable for indentation depth less than 1 μm with conical indenter. Nevertheless, the understanding of the GND density to the surface roughness effect is rarely discussed. Therefore, the present study investigated the relationship dislocation mechanisms in terms of GNDs and surface roughness affect in micro-indentation using finite element analysis. The GND density distribution with surface roughness effect will be revealed.

2. Methodology

2.1 Experimental Method

The single crystal copper (111) with a dimension of 10 mm × 10 mm × 2 mm was purchased for micro-indentation testing. Mechanical polishing with different grit size of 1000, 1500 and 2000 silicon carbide paper was carried out on the specimen to produce three different surface roughness. The surface roughness of the specimen was measured by using surface roughness tester (Mitutoyo Surfiest SV 400). The sampling length to determining the surface roughness parameter on the specimen compliance with EN ISO 4288. 1000, 1500 and 2000 silicon carbide paper resulted a surface roughness of 24 nm, 67 nm, and 140 nm, respectively. Each of the indentation gone through a surface roughness measurement to ensure the indentation had a roughness value that were similar to the roughness of prepared sample.

The micro-indentation was performed by the Sinowan Vickers hardness tester to find out the hardness of the specimen. Before the indentation process, the machine undergone calibration using a calibrator block to indent and tallied the hardness value given in the instrument datasheet. Copper (111) specimen undergone micro-indentation with four different indentation loads of 0.245 N, 0.49 N, 0.9807 N and 1.96 N to observe the indentation size effects response to the various loads. To determine the average hardness of each load, it was performed for five times. Indentation was at least five times farther apart than the size of indentation. The length of diagonal indentation, d was obtained from Vickers hardness tester to calculate the hardness value as expressed in Eq. (1).

$$H = 1.872\frac{F}{d^2} \quad (1)$$

where H is the hardness value and F is the indentation force.

2.1 3D Crystal Plasticity Indentation Model

The 3D indentation model was developed with Abaqus software and the GND density was calculated using the user material subroutine UMAT [12]. The surface roughness of 24 nm, 67 nm, and 140 nm was generated using MATLAB software developed by Kartini *et al.*, [13]. The surface roughnesses was generated on the specimen of indentation model as shown in Figure 1. As copper (111) material was used, Table 1 shows the elastic constants and burger vector of copper (111) material to employ in the finite element simulation.

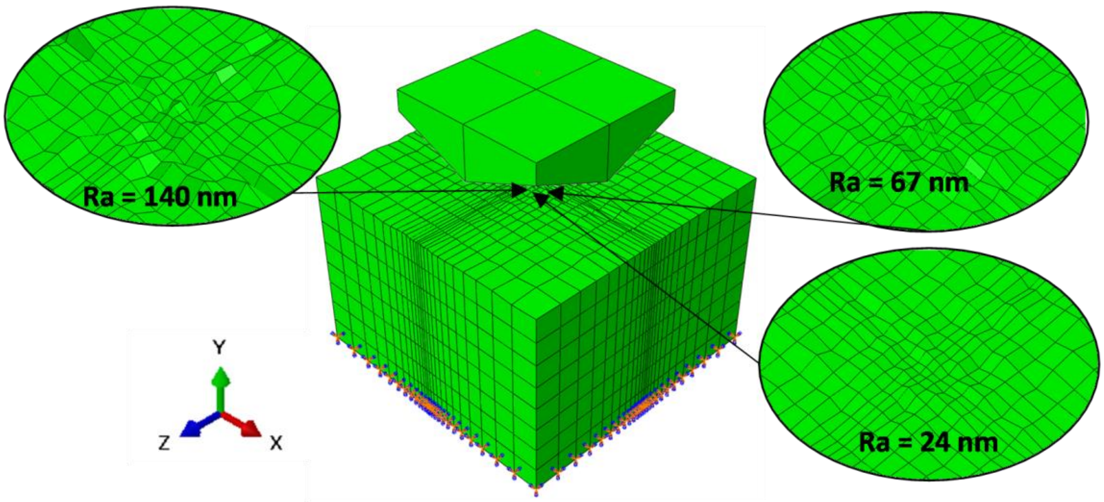

Fig. 1. Various surface roughness was generated on specimen of indentation model

Table 1
The elastic constants and burger vector of copper (111) employed in finite element simulation

Material parameters	
C_{11} [GPa]	168
C_{12} [GPa]	121.4
C_{44} [GPa]	75.4
Burger vector [nm]	0.256

Vickers indenter and the copper (111) specimen were constructed in a dimension of 150 µm × 150 µm × 110 µm as shown in Figure 1. The frictional coefficient between the indenter and specimen was set to zero so that the result of plastic deformation behaviour was solely between the interaction between indenter and surface asperities [5]. The Vickers indenter was set to be rigid. 8,000 quadratic hexahedral element (C3D8) was employed in the model. A fixed boundary condition for all degree of freedom was set to the bottom of specimen. The loading and unloading process was controlled by displacement, h and was set to 3.55 µm, 5.41 µm, 8.25 µm and 12.27 µm. The indenter was applied to travel in y-axis only. The indenter descended for 8 seconds, then dwelled for 10 seconds before returning to its original position. The load-displacement graph was generated to determine the hardness and validate with the experimental hardness value.

3. Results

Load-displacement graph is typically generated from the finite element analysis software to determine the simulation hardness value [14]. As the simulation used displacement method to move the indenter, the indentation depth is represented by the displacement to evaluate the ISE. Figure 2 shows the load against indentation depth graph when h = 3.55 µm, 5.41 µm, 8.25 µm, and 12.27 µm, respectively with varying surface roughness. The rougher surface exhibits a greater indentation load was needed in order to penetrate the material at a given indentation depth. The significant difference of the loading process is due to the presence of surface roughness, which requires flattening surface asperities before penetrating the material [7].

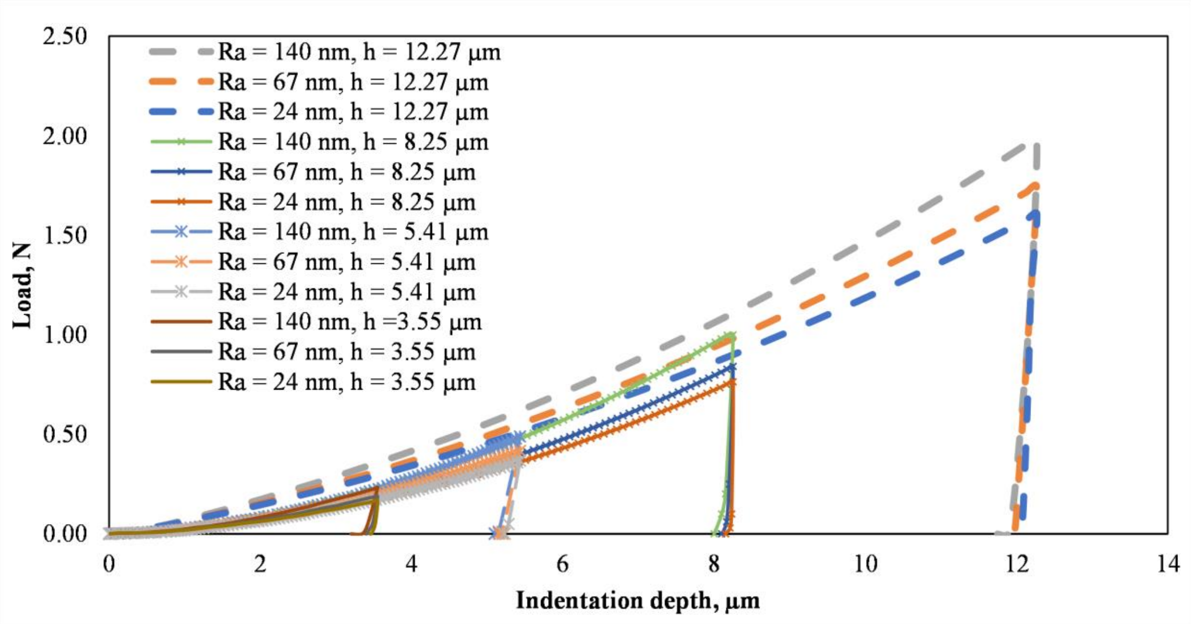

Fig. 2. Load-indentation depth curve obtained from simulation

Figure 3 shows the hardness value of simulation and experiment are plotted against indentation depth. The simulation and experiment hardness value both are in good agreement, indicating the GND density result generated from simulation is reliable. The degree of ISE increases as the surface becomes rougher. The rougher surface tends to have a greater hardness value compared to smoother surface. The roughness effect is more pronounced in small indentation load and gradually decrease as the indentation load increase. Therefore, the hardness is greater for rougher surface.

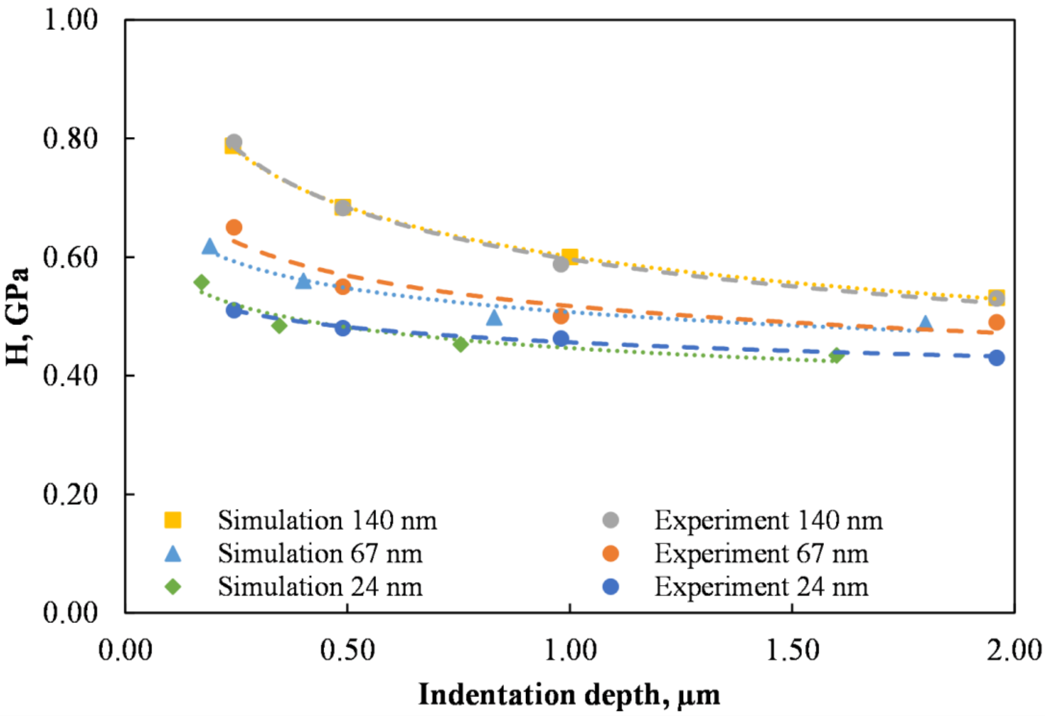

Fig. 3. Hardness against indentation depth with various surface roughness level

Nix-Gao relation revealed the ISE by introducing the presence of hardening effect which is associated with the GND density [2]. Figure 4 shows the surface roughness effect alters the GND density. The GND density increase exponentially with the surface roughness and this behaviour decreases as the indentation depth increase. The trend in Figure 4 fits with Nix-Gao relation. Based on Figure 4, indentation depth of 3.55 µm has the steepest line gradient, which indicates GND density is more pronounced at a lower indentation depth and gets more severe as surface roughness increases.

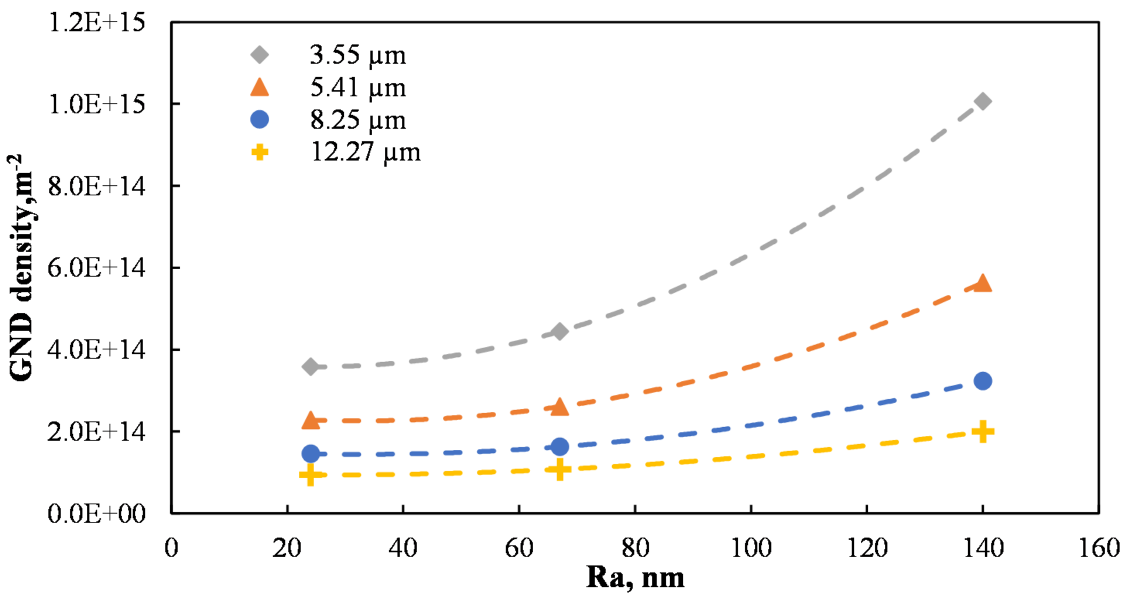

Fig. 4. GND density against surface roughness, Ra with various indentation depth

Figure 5 presents cross-sectional view of the distribution of GND density with surface roughness 24 nm, 67 nm, and 140 nm at indentation depth 3.55 µm and 5.41 µm. The rougher surface resulting GND density exhibits an asymmetric distribution and the maximum GND is generated near the slant of indentation rather than the middle of indentation, where the indenter tip position is [15-16]. This indicates the GNDs are stored at surface asperities and acts as an obstacle to restrict the dislocation motion [17]. Based on Figure 5, the GNDs distribution is highly dependent on the geometry of surface asperities, as the surface get smoother the GND distribution tends to have less inhomogeneous distribution. This is due to GND density is lesser for smoother surface.

Based on Figure 5, it is interesting to note that GNDs volume is smaller for surface roughness 140 nm compared to 24 nm at the same indentation depth. Based on Nix-Gao model, volume of GNDs is inversely proportional to GND density [2]. Therefore, the smaller volume of GND resulting a greater GND density in rougher surface. The GND density decreases as the indentation depth increases. Hence, the distribution of GNDs are lesser for indentation depth, 3.55 µm compared to 5.41 µm. The present analysis shows the same trend with previous studies [2,10].

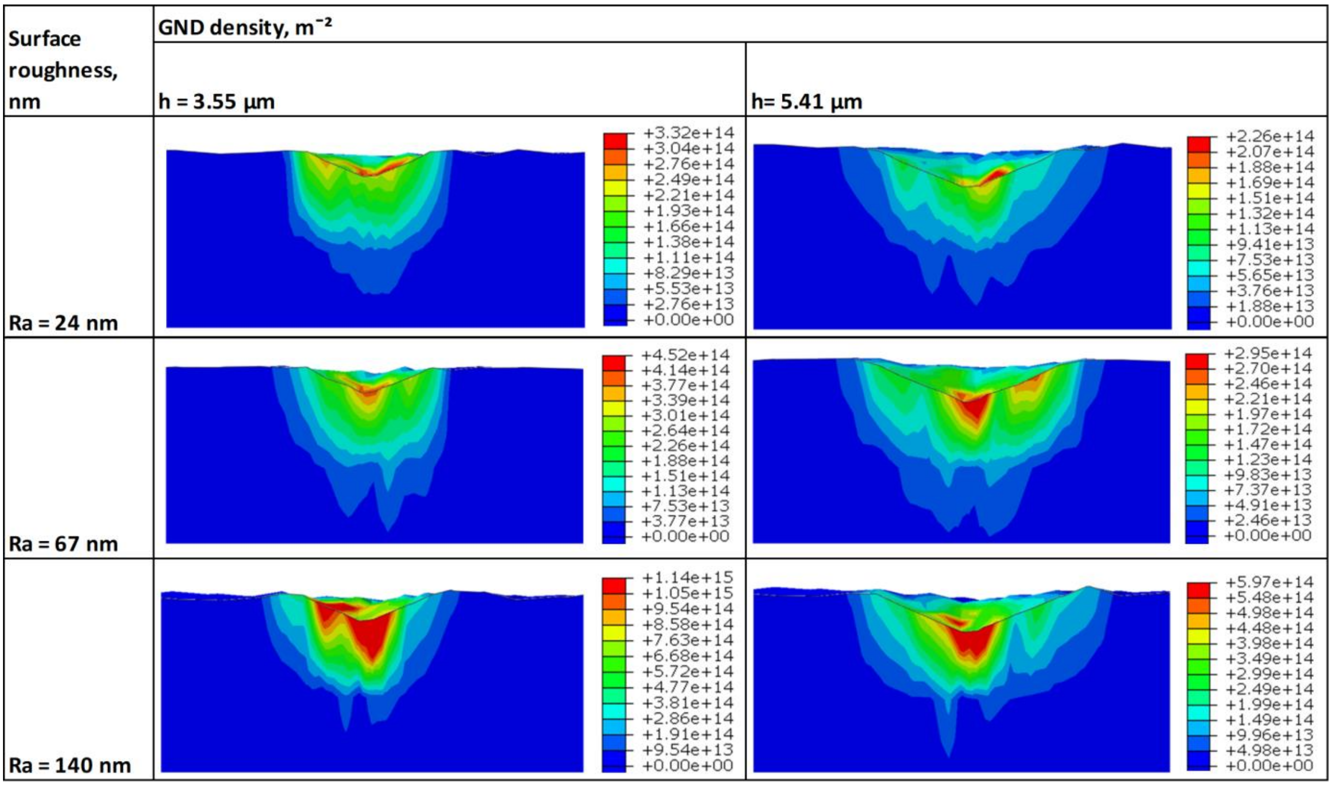

Fig. 5. Cross-sectional view of GND density with various surface roughness and indentation depth

Figure 6 displays cross-sectional view of residual indentation along X axis with various surface roughness when indentation depth is 3.55 µm. The surface roughness with 140 nm revealed to has the most uneven surface at residual indentation compared to surface roughness, 24 nm. This evident shows that the indenter is not completely flattened the surface during the indentation. A portion of the indentation force is used to flatten the surface asperities before indent on the flattened surface for rougher surface [8]. This concluded the surface roughness effect contributed to the hardening effect, leading to the severity in ISE at low indentation depth.

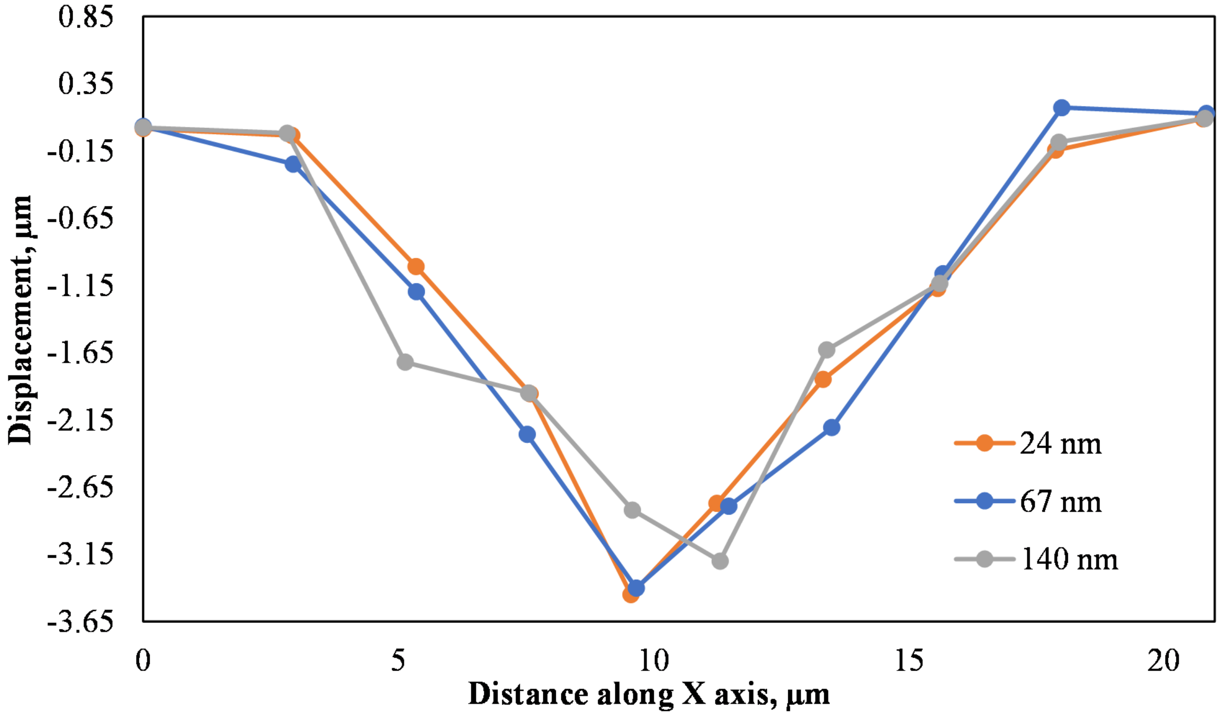

Fig. 6. Cross-sectional view of residual indentation along X axis when indentation depth is 3.55 µm

4. Conclusions

The current study revealed the relationship between the material dislocation through GNDs and surface roughness effect using finite element analysis. Four different indentation depths and three different surface roughnesses were indented on copper (111). Experimental hardness value was compared with simulation hardness value. Finite element simulation was used to obtain GND density. This method quantified the GND density with roughness effect which was responsible for indentation size effect. The following conclusion can be formed based on the findings.

i. Surface roughness plays a role in contributing to GND density and indentation size effect.
ii. The GND density is exponentially proportional to the surface roughness and inversely proportional to the indentation depth.
iii. GND density is distributed inhomogeneously depending on the surface geometry. The GNDs volume varies with surface roughness.

Acknowledgement
This research was funded by a grant from Ministry of Higher Education of Malaysia (FRGS Grant FRGS/1/2018/TK03/KDUPG/03/2).

References
[1] McElhaney, K. W., Joost J. Vlassak, and William D. Nix. "Determination of indenter tip geometry and indentation contact area for depth-sensing indentation experiments." *Journal of Materials research* 13, no. 5 (1998): 1300-1306. https://doi.org/10.1557/jmr.1998.0185
[2] Nix, William D., and Huajian Gao. "Indentation size effects in crystalline materials: a law for strain gradient plasticity." *Journal of the Mechanics and Physics of Solids* 46, no. 3 (1998): 411-425. https://doi.org/10.1016/s0022-5096(97)00086-0

[3] Huang, Y., H. Gao, W. D. Nix, and JW1727555 Hutchinson. "Mechanism-based strain gradient plasticity—II. Analysis." *Journal of the Mechanics and Physics of Solids* 48, no. 1 (2000): 99-128. https://doi.org/10.1016/S0022-5096(99)00022-8

[4] Chen, Ling, Aylin Ahadi, Jinming Zhou, and Jan-Eric Ståhl. "Quantitative study of roughness effect in nanoindentation on AISI316L based on simulation and experiment." *Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science* 231, no. 21 (2017): 4067-4075. https://doi.org/10.1177/0954406216657575

[5] Chuah, Hun Guan, and Zaidi Mohd Ripin. "Modeling of microindentation with consideration of the surface roughness." *Metallurgical and Materials Transactions A* 44 (2013): 5676-5687. https://doi.org/10.1007/s11661-013-1930-5

[6] Jiang, Wu-Gui, Jian-Jun Su, and Xi-Qiao Feng. "Effect of surface roughness on nanoindentation test of thin films." *Engineering Fracture Mechanics* 75, no. 17 (2008): 4965-4972. https://doi.org/10.1016/j.engfracmech.2008.06.016

[7] Kim, Ju-Young, Seung-Kyun Kang, Jung-Jun Lee, Jae-il Jang, Yun-Hee Lee, and Dongil Kwon. "Influence of surface-roughness on indentation size effect." *Acta materialia* 55, no. 10 (2007): 3555-3562. https://doi.org/10.1016/j.actamat.2007.02.006

[8] Tang, Ding, Leilei Zhao, Huamiao Wang, Dayong Li, Yinghong Peng, and Peidong Wu. "The role of rough surface in the size-dependent behavior upon nano-indentation." *Mechanics of Materials* 157 (2021): 103836. https://doi.org/10.1016/j.mechmat.2021.103836

[9] Javaid, Farhan, Yukun Xu, Enrico Bruder, and Karsten Durst. "Indentation size effect in tungsten: quantification of geometrically necessary dislocations underneath the indentations using HR-EBSD." *Materials Characterization* 142 (2018): 39-42. https://doi.org/10.1016/j.matchar.2018.05.016

[10] Qu, S., Y. Huang, W. D. Nix, H. Jiang, F. Zhang, and K. C. Hwang. "Indenter tip radius effect on the Nix–Gao relation in micro-and nanoindentation hardness experiments." *Journal of materials research* 19, no. 11 (2004): 3423-3434. https://doi.org/10.1557/JMR.2004.0441

[11] Demir, Eralp, Dierk Raabe, Nader Zaafarani, and Stefan Zaefferer. "Investigation of the indentation size effect through the measurement of the geometrically necessary dislocations beneath small indents of different depths using EBSD tomography." *Acta Materialia* 57, no. 2 (2009): 559-569. https://doi.org/10.1016/j.actamat.2008.09.039

[12] Grilli, Nicolò, Edmund Tarleton, and Alan CF Cocks. "Coupling a discrete twin model with cohesive elements to understand twin-induced fracture." *International Journal of Fracture* 227 (2021): 173-192. https://doi.org/10.1007/s10704-020-00504-9

[13] Saputra, E., R. Ismail, J. Jamari, and A. P. Bayuseno. "Analysis of the contact area of smooth and rough surfaces in contact with sphere indenter using finite element method." In *MATEC Web of Conferences*, vol. 58, p. 04007. EDP Sciences, 2016. https://doi.org/10.1051/matecconf/20165804007

[14] Najjar, I. M. R., A. M. Sadoun, Ghazi S. Alsoruji, Mohamed Abd Elaziz, and A. Wagih. "Predicting the mechanical properties of Cu–Al2O3 nanocomposites using machine learning and finite element simulation of indentation experiments." *Ceramics International* 48, no. 6 (2022): 7748-7758. https://doi.org/10.1016/j.ceramint.2021.11.322

[15] Han, Qi-Nan, Shao-Shi Rui, Wenhui Qiu, Yue Su, Xianfeng Ma, Zimu Su, Haitao Cui, and Huiji Shi. "Effect of crystal orientation on the indentation behaviour of Ni-based single crystal superalloy." *Materials Science and Engineering: A* 773 (2020): 138893. https://doi.org/10.1016/j.msea.2019.138893

[16] Lewandowski, M. J., and S. Stupkiewicz. "Size effects in wedge indentation predicted by a gradient-enhanced crystal-plasticity model." *International Journal of Plasticity* 109 (2018): 54-78. https://doi.org/10.1016/j.ijplas.2018.05.008

[17] Berahmand, M., M. Ketabchi, M. Jamshidian, and S. Tsurekawa. "Investigation of microstructure evolution and martensite transformation developed in austenitic stainless steel subjected to a plastic strain gradient: A combination study of Mirco-XRD, EBSD, and ECCI techniques." *Micron* 143 (2021): 103014. https://doi.org/10.1016/j.micron.2021.103014