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https://doi.org/10.1140/epjb/s10051-021-00253-1 THE EUROPEAN PHYSICAL JOURNAL B Regular Article - Computational Methods Temperature and indenter radius effects on mechanical properties of copper during nanoindentation: a molecular dynamic simulation study Iwan Halim Sahputraa Industrial Engineering Department, Petra Christian University, Surabaya, Indonesia Received 21 September 2021 / Accepted 16 November 2021 © The Author(s), under exclusive licence to EDP Sciences, SIF and Springer-Verlag GmbH Germany, part of Springer Nature 2021 Abstract. Molecular dynamics simulations of nanoindentation have been performed using a spherical inden- ter that penetrates a surface of an FCC copper model. The effects of the indenter radius and temperature on the mechanical properties and deformation mechanisms are investigated. Several deformation mechanisms, including atomic structural changes, dislocations, and pile-up of atoms around the indenter, are observed depending on the indenter radius and temperature. Increasing the simulation temperature decreases the hardness and reduced modulus. The reduced modulus decreases with the decreasing of the indenter radius while the hardness does not change significantly. 1 Introduction Recently, copper has been used widely in micro- electronic applications. Some examples of its appli- cations are lead frames, interconnection wires, and heat sinks. Considering their important role in the applications, besides the electrical and thermal prop- erties, their mechanical properties are also important to be investigated. Their mechanical properties, such as hardness and stiffness, will influence their overall performance. Nanoindentation becomes a more popular

method to study the mechanical properties of the mate- rial, especially for micro and nano-scale application. Molecular dynamic (MD) simulation has been used intensively along with the experiment, to investigate further the deformation mechanism in microscale dur- ing nanoindentation. Saraev and Miller [1] investigated the deformation mechanism of multi-layered copper thin film during the nanoindentation test. They found that the gliding of nucleated dislocation loops and the slip in the grain boundaries are the main deformation mechanisms in such multi-layered polycrystals. Liang et al. [2] studied the deformation behaviour in the three different crystallographic orientations of copper under nanoindentation. They found a yielding plat- form attributed to the effective resistance to dislocation locks in the load-displacement curve of copper oriented (001). While in copper oriented (111) and (110) more mobile dislocation structures are found as typical char- acteristic causes of load drops in the load–displacement curves. Fang et al. [3] investigated the effect of veloc- a e-mail: iwanh@petra.ac.id (corresponding author) 0123456789().: V,-vol ity and loading on the nanoindentation of the copper thin film. They found that both Young's modulus and hardness increase up to a critical value of indentation velocity and decrease after that value. Young's modu- lus decreases, but hardness increases as the indentation load increases. In the micro- and nano-scale application of copper material, surrounding temperature and contact area to other components are also important factors that can influence the mechanical properties. Zhao et al. [4] presented temperature-dependent mechanical prop- erties of single-layer molybdenum disulphide obtained using MD nanoindentation simulations. The Young's moduli, maximum load stress, and maximum loading strain decrease with increasing temperature from 4.2 to 500 K. Guo et al. [5] reported the effect of tem- perature on the nanoscale deformation behaviour and mechanical properties of c-plane monocrystalline gal- lium nitride under nanoindentation. It was found that both the hardness and Young's modulus decreased as the temperature increased. Similar results were also found by Fang et al. [6], however, their estimated elas- tic moduli and hardness are much higher than the prior experiments. In this paper, the effects of the indenter radius as a representative of the contact area and sim- ulation temperature on the mechanical properties and deformation mechanisms of copper during nanoinden- tation are evaluated and reported. 2 Methods The copper sample used in the simulation contains 6806 atoms and the dimension is 148.215 × 148.215 × 3.615 Table 1 Elastic constants for Cu Method C11 (GPa) C12 (GPa) C44 (GPa) EAM-Adams [7] 168.1 123.7 78.8 Experiment [10] 168.4 121.4 75.4 Fig. 1 Displacement versus time set up to control the indenter movement Å3. The Boundary conditions in x- and z-directions are set to be periodic for simulating an infinite length in these directions. In y-direction, a shrink-wrapped boundary condition is set up to simulate a free sur- face where the indentation tip is located. Some atoms at the bottom in the y-direction are held fixed during indentation. The EAM potential for Cu from Adams et al. [7] is used in this simulation. The embedding functions are determined empirically by fitting to several measured parameters, namely the equilibrium lattice constant, sublimation energy, and bulk modulus, elastic con- stants, and vacancy formation energy [8]. The advan- tage of the EAM potential model is it combines the computational simplicity needed for a large model with a physical picture that includes many-atom effects and metallic bonding [9]. The elastic constants of Cu calcu- lated using this potential are in good agreement com- pared to experimental values [10] as shown in Table 1. Nanoindentation is performed using a spherical indenter into a [010] surface of the FCC copper sam- ple. The velocity of the indenter is set up to be 0.15 Å/ps, and the displacement is controlled following the displacement versus time pattern given in Fig.1. After reaching the maximum deformation, the indenter is held still for a moment before unloading started. This is usually done in the nanoindentation test to let the instrument and specimen stabilise and also to measure creep within the specimen [11]. Fang et al. [3] have shown in the MD simulations of nanoindentation, both Young's modulus and hard- ness increase up to a critical value of indentation veloc- Fig. 2 Load versus indentation depth of Cu with indenter radius 10 lattice length at 5 K ity (80 m/s) and decrease after that value. Imran et al. [12] presented the increase of hardness with indentation velocity from 10 to 200 m/s. In the other MD simula- tions of nanoindentation, Goel et al. [13] indicated that Young's modulus does change significantly in the range of indentation velocity between 5 and 100 m/s. In this work, the indentation velocity is set to be a constant parameter, to investigate the effect of temperature and indenter radius. The first part of the simulation is done using five dif- ferent radiuses that are 5, 10, 15, 20, and 25 in lattice units at temperature 25 K. Lattice unit means that the unit is given in the unit cell size, which in this sim- ulation is 3.615 Å. Before indentation, the sample is relaxed at the desired temperature. The second part of the simulation is done using indenter radius ten lattice units with five different temperatures that are 5 K, 25 K, 45 K, 65 K, and 85 K. Common neighbour analysis (CNA) [14] is performed during the simulation to study the change in the crystal structure. Using this analysis technique, various local crystal structures, especially FCC, HCP, BCC, and icosahedral, can be distinguished. Simulation is done using a classical molecular dynamics program called LAMMPS [15] and an atomistic visualisation program OVITO [16] is used to visualise the simulation result. The calculation and analysis procedures are done fol- lowing the technique proposed by Oliver and Pharr [17]. After performing the nanoindentation simulation, the initial unloading stiffness (S) is calculated. The relationship between load and depth from unloading data for stiffness calculation is described using a simple power law: $P = A(h - hf)m$, (1) where A and m are constants and hf is the residual depth after the unloading process. The curve fitting method used is nonlinear least squares with the trust- (a) (b) (c) Fig. 3 CNA Visualization and von Mises stress contour at some interesting points during indentation with an indenter radius 10 lattice units at the temperature of 5 K region algorithm which is in the curve fitting tool of The displacement of the surface at the contact the MATLAB program ver. 7.10.0. The initial slope, or perimeter, hs, is calculated by: stiffness (S), is calculated first by differentiating that equation analytically and then calculating the deriva- tive at the peak load and displacement: $hs = \varepsilon Pmax . S$ (3) $\varepsilon S = dh = mA(h - hf) dP m-1 .$ (2) The value of used in this analysis is 0.75, S is cal- culated from Eq. (3), and Pmax is from data. Fig. 4 Load versus indentation depth with various temperatures in K (a) and indenter radius in lattice units (b). Note. For R = 10 lattice units and T = 85 K: (*) at time = 78 ps and depth = 11.7 Å, (**) at time = 80 ps and depth = 12Å, (***) at time = 82 ps and depth 12 Å The contact depth, hc, is determined by: $hc = hmax - hs.$ (4) The projected contact area of spherical indenter tip at peak load is computed using the following equation: $A = 2\pi rihc,$ (5) where ri is the radius of the indenter. The reduced modulus, Er, is calculated by: $\sqrt{\pi S} Er = 2 \sqrt{} . A$ (6) And the hardness of the specimen is calculated by: $H= Pmax A ,$ (7) where Pmax is the peak indentation load and A is the projected area of the hardness impression. The reduced modulus (Er) is also calculated using Hertz elastic contact model [18] as: $P= 4 Erh3/2r1/2, 3$ (8) where P is the load, r is the indenter radius, and h is the indentation depth. The reduced modulus value is obtained from the values for indentation depth (h) of 1 Å and 2 Å. 123 3 Result and discussion 3.1 Deformation analysis The load (P) versus indentation depth (h) of nanoin- dentation on copper using an indenter radius of 10 lat- tice units

(i.e., 36.15 Å) at a temperature of 5 K is pre- sented in Fig. 2. The first BCC structure formed during the indentation is observed at the depth of 6.6 Å as shown in Fig. 3a-left. At around this depth, the load curve is steady as indicated at point 'A' in Fig. 2. The von Mises stress in the region where the struc- tural changes happen and its nearby is higher than in another region, as can be seen in Fig. 3a-right. Sev- eral atoms right beneath the indenter have lower von Mises stress. The high-stress region develops symmet- rically about the y -axis at 45◦ angle from the inden- tation point. The region area containing atoms having BCC structure continues to grow until the maximum displacement (12 Å) of the indenter. After the indenter reaches the maximum depth at 80 ps and is kept at that position for 5 ps, the load decreases and indicates relaxation behaviour. During this period, atoms having HCP structure are observed at 84 ps, as presented in Fig. 3b-left, which is corre- sponding to the point 'B' in Fig. 2. Dislocation is started to be nucleated at the boundary of the region having HCP structure and unknown structure and then trans- mitted along the [110] direction. The von Mises stress contour is still symmetric about the y -axis as presented in Fig. 3b-right. At the depth around 8 Å corresponding to the point 'C' in Fig. 2, the load is steady, then followed by a sud- den drop of the load. This is related to Fig. 3c-left, the region previously having HCP structure changes to having BCC structure. The atoms having unknown structure and dislocations move along [110] direction. In addition to that, it can be seen the atoms with unknown Fig. 5 Temperature and indentation radius effects on the deformation mechanisms. Green dots = atoms having BCC structure, blue dots = atoms having HCP structure, red dots = atoms having unknown structure. Only atoms having non-FCC structure are shown for clarity structure have higher von Mises stress as presented in Fig. 3c-right. After the sudden drop, the load then decreases smoothly with a similar shape to the loading process. When the indenter is completely removed from the sam- ple, as presented in Fig. 2, small plastic deformation is observed. From Fig. 5 (R =10 lattice units, T = 5 K, Time = 165 ps), which will be discussed further in the next section, it can be seen at the end of the simu- lation some atoms having unknown structure are still observed. 3.2 Effect of temperature and indenter radius Temperature does not make much change on the shape of the load-depth curve as presented in Fig. 4a. Lower temperature slightly shifts the curve up since lower tem- perature reduces the mobility of the atoms and makes them more difficult to be deformed. A comparison of the deformation mechanisms for the simulations with temperatures of 5 K and 85 K is shown in Fig. 5 with an indenter radius of 10 lattice units. In this figure, only atoms having non-FCC structure are shown for clarity. Atoms located at the top and bottom layers of the sim- ulation box have unknown structure because of a non- periodic boundary condition applied to this direction. At the simulation with a temperature of 85 K, atoms having HCP structure are observed at an earlier time (at 80 ps) than at the simulation with a temperature of 5 K (at 84 ps). The region having unknown structure are recovered back to have FCC structure more quickly in the simulation with a temperature of 85 K than in the simulation with a temperature of 5 K. This shows the effect of temperature on the deformation behaviour, structural change happens easier at a higher tempera- ture Fig. 6 Temperature effect on the hardness (a) and reduced modulus (b) Fig. 7 Indenter radius effect on the hardness (a) and reduced modulus (b) Figure 4b shows the effect of the indenter radius vari- ation on the load-depth curve. The loading and unload- ing curves of the simulations using an indenter radius larger than 10 lattice units are almost on top of each other. At the simulations using an indenter radius larger than 10 lattice units, the load drop when the indenter stops after reaching the maximum depth, is less than in the simulation using a smaller indenter radius. The simulation using an indenter radius of 5 lat- tice units shows the decreasing of the load when the depth increases during the loading process after the depth of about 9 Å, as presented in Fig. 4b. During the load decreasing process, the dislocation movement is observed along the [100], [110], and [110] directions. This load decreasing behaviour is similar to the strain- softening phenomenon observed by Champion et al. [19], Haouaoui et al. [20], and Li et al. [21] in ten- sile and compressive tests for copper nanocrystalline or ultrafine-grained with grain sizes of 50–400 nm. Nanoindentation using a smaller indenter radius (especially with a radius of 5 lattice units) shows plas- tic behaviour, while using a larger indenter radius tends to show elastic behaviour. As shown in Figs. 4b and 5 (R = 5 lattice units, Time = 165 ps), using an indenter with radius 5 lattice units, after the indentation is com- pletely removed from the sample, small deformation is still observed. A significant pile-up of atoms around the indenter is observed during the indentation process even after the indenter has been completely removed from the sample (depth = 0 and time = 165 ps). Simulation using the largest indenter radius i.e., 25 lattice units, does not show a pile of atoms and the contour of the surface is completely recovered at the end of the simu- lation as shown in Fig. 5 (R = 25 lattice units, Time = 165 ps). The effect of temperature on the hardness and reduced modulus is shown in Fig. 6a, b. It can be seen in Fig. 6a, decreasing the temperature causes the hardness to increase. Krashchenko and Oksametnaya [22] using rigid rectangular pyramid sapphire indenter showed that the decreasing of the hardness of pure cop- per as the temperature testing increases from 290 to 1170 K. The similar trend also found by Huang et al. [23], the hardness decreases from 4.4 to 0.8 GPa as the temperature increases from 83 to 333 K. Our predicted hardness at 85 K is close to these experimental values. Reduced modulus calculated using the Hertz model with 1 Å depth is closer to the value calculated using Oliver and Pharr (OP) model compared to the value calculated using the Hertz model with 2 Å depth as shown in Fig. 6b. The reduced modulus shows the same behaviour as the hardness, it decreases as the tempera- ture increases. Lebedev et al. [24] experimentally found Young's modulus for copper of approximately 116–126 GPa at the range of temperature of 473 K and 293 K. Our predicted modulus calculated using the OP model is close to these experimental values. Using the smallest radius of indenter (5 lattice units) produces a lower hardness value than the larger one (10 lattice units) as shown in Fig. 7a. But then the hardness values decrease along with the increase of the inden- ter radius. However, the values, except for the indenter radius of 10 lattice units, are not significantly different. Qiu et al. [25] also showed that different indenter radius almost has no effect on the hardness of the material in the MD nanoindentation simulation amorphous alloy. They used various radii of indenter of 3.0, 3.5, 4.0, and 4.5 nm. Increasing indenter radius makes the reduced modu- lus decreases as presented in Fig. 7b. This is related to the change in the atomic structure during the indenta- tion. In Fig. 5, the simulation using an indenter radius of 5 lattice units shows fewer atoms undergo a struc- tural change from FCC to BCC compared to the sim- ulation using an indenter radius of 25 lattice units at the same temperature. Furthermore, there is no change from FCC structure to HCP structure is observed dur- ing the nanoindentation using an indenter with 5 lat- tice units radius. Fang et al. [3] using MD simulation showed that Young's modulus decrease as the penetra- tion depth increases. A Larger indenter radius means deeper penetration depth of the indenter; therefore, the modulus is reduced. 4 Conclusion Molecular dynamic simulations of nanoindentation on copper have been performed using different inden- ter radius and at different temperatures. Deforma- tion mechanisms, including structural changes, dislo- cations, and pile-up of atoms around the indenter, are observed depending on

the indenter radius and temper- ature. Increasing the temperature decreases the hard- ness and reduced modulus. Hardness does not change significantly with the reduction of indenter radius. The reduced modulus decreases with the decreasing of indenter radius. The predicted Young's modulus and hardness are close to previous measurements. Data Availability Statement This manuscript has no associated data or the data will not be deposited. [Authors' comment: The data that support the findings of this study are available from the corresponding author, upon reason- able request.] References 1. Denis Saraev, Ronald E. Miller, Model. Simul. Mater. Sci. Eng. 13, 1089 (2005) 2. H. Liang, C.H. Woo, H. Huang, A.H.W. Ngan, T.X. Yu, Science 6, 105 (2004) 3. Te-Hua. FANG, Sheng-Rui. JIAN, Der-San. CHUU, pn. J. Appl. Phys. 41, L 1328 (2002) 4. Junhua Zhao, Jin-Wu. Jiang, Timon Rabczuk, Appl. Phys. Lett. 103, 231913 (2013) 5. Jian Guo, Jingjing Chen, Yongqiang Wang, Ceram. Int. 46, 12686 (2020) 6. Te-Hua. Fang, Cheng-I. Weng, Jee-Gong. Chang, Mater. Sci. Eng., A 357, 7 (2003) 7. J.B. Adams, S.M. Foiles, W.G. Wolfer, J. Mater. Res. 4, 102 (1989) 8. S.M. Foiles, M.I. Baskes, M.S. Daw, Phys. Rev. B 33, 7983 (1986) 9. M.S. Daw et al., Mater. Sci. Rep. 9, 251 (1993) 10. T. Zhu, J. Li, K.J. Van Vliet, S. Ogata, S. Yip, S. Suresh, J. Mech. Phys. Solids 52, 691 (2004) 11. Anthony C. Fischer-Cripps, Nanoindentation Testing (Springer, New York, 2011) 12. Muhammad Imran et al., Chin. Phys. B 21, 116201 (2012) 13. Saurav Goel et al., J. Phys. D Appl. Phys. 47, 275304 (2014) 14. Daniel Faken, Hannes Jónsson, Comput. Mater. Sci. 2, 279 (1995) 15. S.J. Plimpton, J. Comput. Phys. 117, 1 (1995) 16. A. Stukowski, Model. Simul. Mater. Sci. Eng. 18, 015012 (2010) 17. W.C. Oliver, G.M. Pharr, J. Mater. Res. 7, 1564 (1992) 18. K.L. Johnson, Contact Mechanics (Cambridge Univer- sity Press, Cambridge, 1985) 19. Yannick Champion, Cyril Langlois, Sandrine Guérin- Mailly, Patrick Langlois, Jean-Louis. Bonnentien, Mar- tin J. Hÿtch, Science 300, 310 (2003) 20. M. Haouaoui, I. Karaman, H.J. Maier, K.T. Hartwig, Metall. Mater. Trans. A 35 A, 2935 (2004) 21. Y.J. Li, W. Blum, F. Breutinger, Mater. Sci. Eng., A 387–389, 585 (2004) 22. V.P. Krashchenko, O.B. Oksametnaya, Strength Mater. 16, 209 (1984) 23. Z. Huang, L.Y. Gu, J.R. Weertman, Scripta Mater. 37, 1071 (1997) 24. A.B. Lebedev, Yu.A. Burenkov, A.E. Romanov, V.I. Kopylov, V.P. Filonenko, V.G. Gryaznov, Mater. Sci. Eng., A 203, 165 (1995) 25. Chen Qiu, Pengzhe Zhu, Fengzhou Fang, Dandan Yuan, Xuecen Shen, Appl. Surf. Sci. 305, 101 (2014)