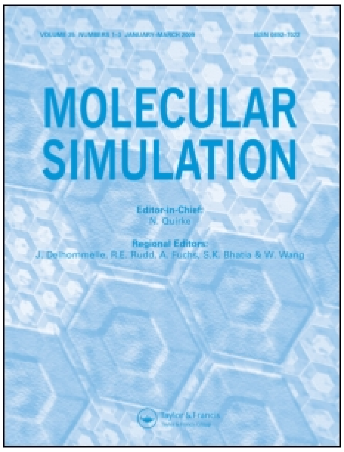

Molecular Simulation
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713644482

A straw model simulating nanoindentation

S. Mukherjee[a]; S. Murray[a]; T. Khraishi[a]; Y. -L. Shen[a]
[a] Department of Mechanical Engineering, University of New Mexico, Albuquerque, NM, USA

To cite this Article Mukherjee, S. , Murray, S. , Khraishi, T. and Shen, Y. -L.(2006) 'A straw model simulating nanoindentation', Molecular Simulation, 32: 5, 339 — 343
To link to this Article: DOI: 10.1080/08927020600752431
URL: http://dx.doi.org/10.1080/08927020600752431

Molecular Simulation, Vol. 32, No. 5, 30 April 2006, 339–343

Taylor & Francis
Taylor & Francis Group

A straw model simulating nanoindentation

S. MUKHERJEE, S. MURRAY, T. KHRAISHI* and Y.-L. SHEN

Department of Mechanical Engineering, University of New Mexico, Albuquerque, NM 87131, USA

(Received February 2006; in final form April 2006)

In this work, we introduce a new model, based on straws, to simulate nanoindentation in a close-packed atomic plane as an alternative to the Bragg–Nye bubble raft model. Upon indentation, our results match quantitatively and/or qualitatively the Bragg–Nye and the atomistic computer simulation models. The straw model also explains the apparent physical cause for the formation of slip-steps or pile-ups at the free surface of the indented material. Finally the model can simulate plane-stress or plane-strain conditions.

Keywords: Nanoindentation; Dislocations; Plastic deformation; Crystal plasticity

1. Introduction

In the Bragg–Nye bubble raft model [1], the crystal structure of a metal is represented by an assemblage of soap bubbles floating on glycerin. These two-dimensional (2D) crystals show structures that exist in metals, and simulate features such as grain boundaries, dislocations, and other types of fault, slip, recrystallisation, annealing and strains due to presence of foreign atoms. When a single crystal or a polycrystalline raft is compressed, extended, or otherwise deformed it exhibits a behavior very similar to that of metals subjected to strain. Irregularly sized bubbles caused a large number of them to be present at the grain boundary. When under the influence of any external force, the model is elastic up to a certain limit beyond which it yields by slip along one of the three equally inclined directions of close-packed rows. Other types of faults, similar to the letter "V", triangles and also holes appear in the crystal structure.

The Bragg–Nye bubble-raft model and its extension were also used to simulate defect nucleation in a crystal during nanoindentation [2,3]. It was observed that homogenous defect nucleation occurs within a crystal when its surface roughness is comparable to the radius of the indenter tip and that the depth of the nucleation site below the surface is proportional to the half-width of contact. It was explained that the first displacement burst generally occurs when maximum shear stress generated under the indenter is of the order of the theoretical shear strength. A dislocation dipole nucleated beneath the indented surface, along the loading axis, at a depth of 0.78 times the half width of contact. One dislocation glided into the crystal and the other ran to the surface creating a slip-step.

Our straw model is an alternative to the Bragg–Nye bubble raft. It aims to offer a macroscopic 2D approximation of nanoindentation, which can be observed *in-situ*, and subsequent defect nucleation. The model includes an array of approximately 3700 straw pieces (53 rows and 69 columns), each 1 in. long (± 0.02 in.) and coated with glycerin on the exterior surface. Note that the number of straws depends on the geometry of the housing, where they were packed, to form a (111) FCC close-packed plane. Glycerin mimics the interatomic forces between atoms and helps to hold the straws together [1]. A cylindrical indenter indents the assemblage from the top at a chosen rate of 0.01 in. per minute till defect nucleation takes place. The observed results show similarity, qualitatively and/or quantitatively, to the observations of the Bragg–Nye model [1] and nanoindentation simulation models [2,4]. Our straw model, in addition to being experimental, *in-situ* and allowing different ratios of atom-to-indenter sizes, as in the previous models, also has the following advantages:

- It is easier, faster and cheaper to set up.
- No bias in tension which means all our atoms are coated with glycerin on all sides whereas in the

*Corresponding author. Tel: 1 505-277-6803. Email: khraishi@me.unm.edu

Molecular Simulation
ISSN 0892-7022 print/ISSN 1029-0435 online
http://www.tandf.co.uk/journals
DOI: 10.1080/08927020600752431

Bragg–Nye model, the bubbles were only wetted by glycerin solution from one side (i.e. where they were in contact with the glycerin solution).

- Can control the degree of tension by varying the amount of glycerin wetting.
- There is minimum "size irregularity" in the straw setup due to equal straw sizes whereas in the Bragg–Nye model, an exact bubble size is difficult to achieve.
- The straw model can simulate plane-stress or plane-strain conditions by varying the length of the straws. The effect of varying the straw length is to vary the interatomic potential and frictional forces between straws. This variation is what actually changes the stress state between plane-stress and plane-strain.

Finally, it is also possible to record a load-displacement curve for the suggested straw model, similar to real nanoindentation experiments. The presented results below do not show such a curve due to the large load-cell attached to our instrumentation. Future plans revolve on obtaining a smaller load-cell capable of accurately recording the small forces involved in indenting the straw model.

2. Method

The housing for the constructed straw model is a $\frac{1}{4}$ in. clear acrylic material (Plexiglas) bonded with strong PVC glue (figure 1). The box is approximately, 17.5 in. tall, 18.25 in. wide and 5 in. deep. These dimensions can change if one wants to house more straws or longer/shorter ones. The straws have a diameter of 0.26 in. each. If the straws were modeling an FCC metal such as Copper, then the scale would be approximately 2.58×10^7 to 1. Once the final housing was built, a total of 3657 straws, each of approximate length 1 in. ($\pm$ 0.02 in.) was manually cut and measured. Straws were cut using a regular paper cutter. These straws were then measured for length accuracy using a digital caliper. The straws were individually grabbed using tweezers, surface dipped in glycerin solution and then stacked side by side to form a layer of 69 atoms. The next layer of atoms was placed such that they occupied the "valley positions" of the atoms of the first layer. Thus the whole assembly was built up ensuring that there was no room for any atoms to roll and that they were tightly packed at the end walls of the housing. Thus we have a situation where the packing has only the top surface as a "free surface" and the other three sides do not allow any atom movement perpendicular to them. A tensile/compression Instron machine then lowers the cylindrical indenter at a chosen rate of 0.1 in. per minute until plasticity became apparent in the model.

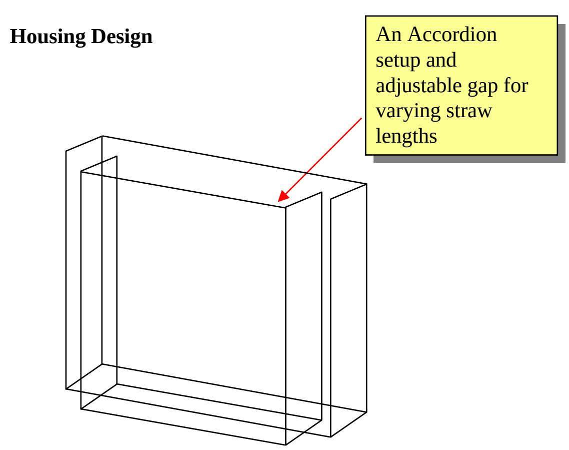

Figure 1. The 1 in. straws were dipped in glycerin and arranged into the slot indicated in the figure. The movements of the straws were restricted from all sides except the top where eventually all the slip-steps and pileups occurred.

Figure 2. Indentation experiment setup, with the cylindrical indenter at the top, on an Instron machine. The indentation is done at a chosen rate of 0.1 in. per minute by pushing down the cylindrical indenter.

An assembly view of the housing design along with the straws is shown in figure 2.

The straws simulate atoms in nanoindentation experiments and the glycerin mimics the interatomic forces, which helps hold the atoms together. The tension effects of glycerin has been tested and found to hold for many days.

The indenter for the nanoindentation experiment is cutout from an 8 in. cylinder with a width of approximately 1 in. to match the length of the straws and thus model 2D conditions.

The cylindrical indenter is attached to the jaw of the Instron machine through a metallic pin. A digital video camera was used to record all the experiments in order to ensure that the results are available for post experiment analysis and review. The camera view was setup perpendicular to the plane of the straws.

3. Results and discussion

The indentation setup in figure 2 was used for our experiments. As indentation progressed, at a chosen rate of 0.01 in. per minute, the top layer of atoms were initially compressed beneath the indenter and the array of straws was deforming elastically up to a certain limit (figure 3). On further indentation, significant movement of atoms

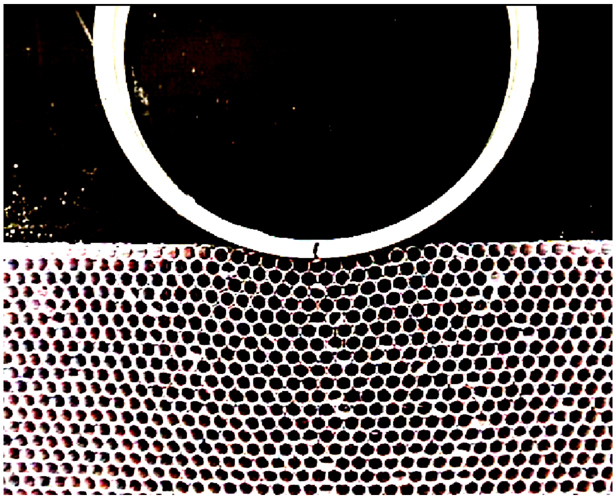

Figure 3. This shows the close-packed plane of atoms undergoing elastic deformation. The cylindrical indenter pushes into the atomic plane, but up to this moment no defects have nucleated.

occurred as dislocations were created. Dislocations moved initially along "V"-shaped tracks (figure 4). These "V" shapes conform to observation from the Bragg–Nye bubble raft model [1]. The preferred movement of dislocations is along the slip directions with the supposed highest resolved shear stress [2,4,5,6]. It was observed that the preferred slip directions are along the 60 and 120° inclinations and the two dislocation slip paths have a 60° angle between them as observed in the earlier models [1,4].

On further indenting the array, it was observed that the dislocations impinge on the free surface and form either slip-steps (figure 5), conforming to observations from the nanoindentation simulation experiments on the Bragg–Nye bubble raft [2,5], or as pile-ups (figure 6), as observed in multi-scale indentation of metals [7,8,9] and in finite element simulation models [10]. We observed that as we increase the amount of glycerin coating the straws, the tendency for pile-ups, as opposed to slip-step formation, at the free surface increases. The reason for this tendency can be attributed to increased inter-atomic cohesion and reduced friction (this tendency is hard to precisely control in our experiments). Friction, like strain hardening, has a significant influence on the piling-up or sinking-in behavior of materials [10]. It has also been stated therein that the existence of friction decreases the piling-up for materials with the tendency to pile-up or increases the sinking-in for materials with the tendency to sink-in. Our straw model represents a material with the tendency to pile-up and hence as friction decreases (with an increase in the amount of glycerin coating straws) the tendency of pile-up increases. The other observation of interest is the formation of holes and triangles in these indentation/compression experiments (figures 5 and 6). This again conforms to the observations of the Bragg–Nye bubble raft model [1] where similar kinds of holes appear and disappear when the crystal is cold-worked.

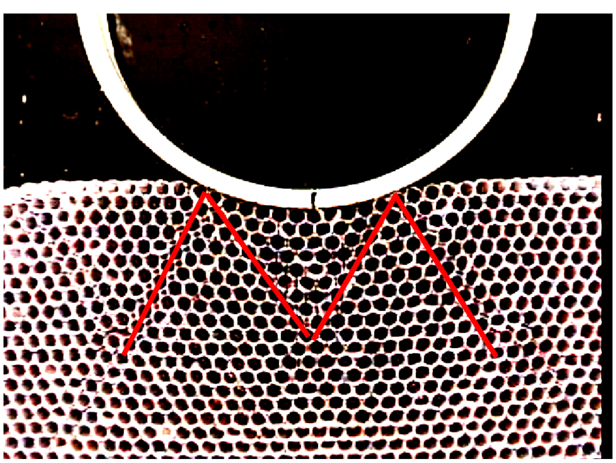

Figure 4. Onset of plasticity where we clearly see the "V" shape. The "V" structure is formed by the dislocation forming inside the structure and then reflecting off of the indenter.

3.1 Comparison of straw model to atomistic modeling

Defect nucleation during nanoindentation was simulated using computer atomistic simulations by our research group [4]. This simulation was done within the 2D framework featuring a model crystal having a close-packed lattice structure, similar to the straw model. The atomistic model defines a close-packed rectangular planar crystal, with one of its close-packed direction parallel to the top surface to be indented. The crystal contains a total of 9525 atoms. Indentation loading with a circular tip is applied to the top surface. The two side boundaries are constrained to remain fixed in their x-positions during indentation, i.e.

$$u_x|_{\mathrm{left}} = u_x|_{\mathrm{right}} = 0,$$

where u_x is the horizontal displacement and the subscripts "left" and "right" represent, respectively, the leftmost and rightmost columns of atoms. The y-direction movements of these boundaries are not restricted. The bottom boundary atoms are not allowed to go in the negative y-direction, i.e.

$$u_y|_{\mathrm{bottom}} \geq 0,$$

while their u_x are unrestricted. This effectively means free sliding of atoms at the interface between the crystal and its underlying rigid substrate. The top surface is unrestrained everywhere except directly under the indenter.

The Morse interatomic potential used is:

$$V = -V_0[\mathrm{e}^{-2a(r-r_0)} - 2\mathrm{e}^{-a(r-r_0)}]$$

Where r is the interatomic spacing and the parameters r_0, a and V_0 are determined by fitting to experimental data of the equilibrium lattice parameter, cohesive energy and bulk modulus of copper featuring near-neighbor interactions [11]. The parameters thus obtained via such fitting are: $r_0 = 2.56$ Å, $a = 1.399$ Å^{-1} and $V_0 = -0.581$ eV.

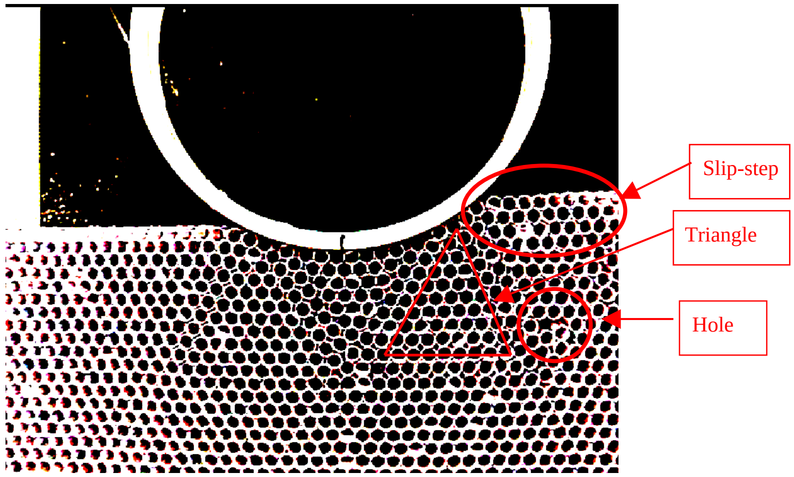

Figure 5. On the right side are some features observed in the experiments such as slip-steps, holes and triangles.

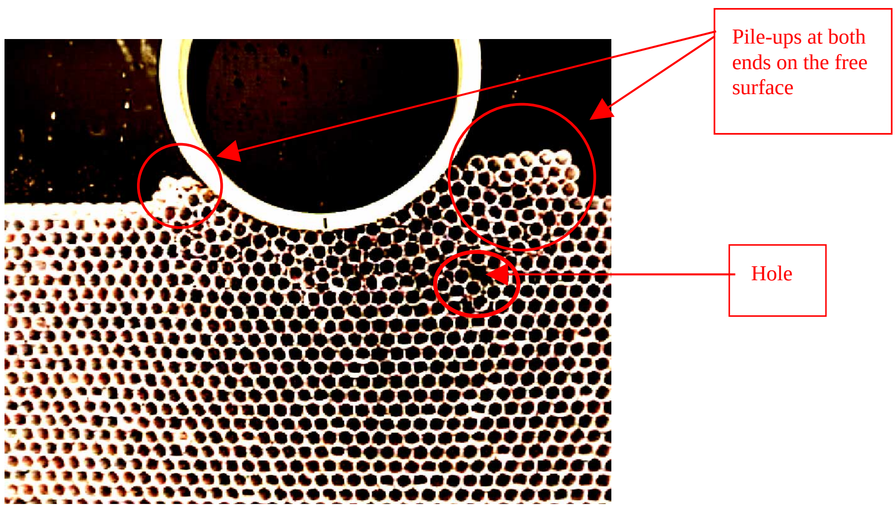

Figure 6. Pile-ups seen on both sides when the amount of glycerin is increased.

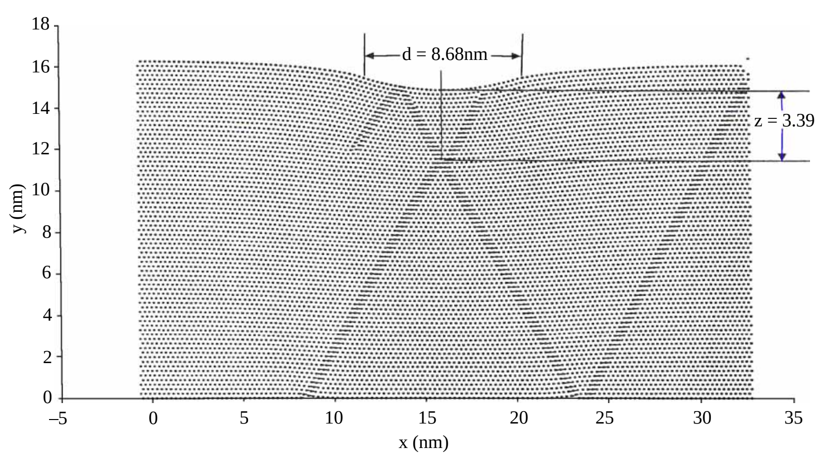

Figure 7. The tracks indicate that two pairs of dislocations have formed and traveled through the material.

Upon indentation, the atomic configuration of the material, soon after the first dislocation nucleation event, is as shown in figure 7 below.

The dislocation tracks, shown by dashed lines, indicate that the apparent depth of dislocation nucleation along the indentation axis is consistent with the location of maximum shear stress predicted using 2D Hertzian contact theory. The tracks also indicate that two pairs of dislocations have formed and traveled through the material. The dislocation movement tracks in figure 7 are consistent with the "V" shapes in our straw model (figure 4).

4. Conclusions

We conclude that our indentation model, based on glycerin-coated straws arranged to form a close-packed (111) FCC plane, can simulate the observations from earlier models like the original Bragg–Nye bubble raft model, the nanoindentation bubble-raft model and the computer atomistic simulation model. Besides being easier, faster and cheaper to setup, it also furnishes an explanation for the preferred formation of slip-steps or pile-ups. Moreover, this model can be used to simulate plane-strain or plane-stress conditions by modifying the setup geometry. It is important here to realize that the similarities observed between the presented straw model and the bubble-raft model are due to the fact that both models simulate a near plane-stress condition since the out-of-plane dimension is much smaller than the in-plane dimensions (with all loads being in-plane as well). Finally, the presented straw model is capable, similar to the bubble-raft model, of simulating polycrystalline or amorphous material by distributing the straws accordingly.

References

[1] W.L. Bragg, J.F. Nye. A dynamic model of a crystal structure. *Proc. R. Soc. Lond. A*, **190**, 474 (1947).

[2] A. Gouldstone, K.J. Van Vliet, S. Suresh. Simulation of defect nucleation in a crystal. *Nature*, **411**, 656 (2001).

[3] V.R. Thalladi, A. Schwartz, J.N. Phend, J.W. Hutchinson, G.M. Whitesides. Simulation of indentation fracture in crystalline materials using mesoscale self-assembly. *J. Am. Chem. Soc.*, **124**, 9912 (2002).

[4] R.W. Leger, Y.-L. Shen, T.A. Khraishi. Defect nucleation during nanoindentation: an atomistic analysis. *J. Comput. Theor. Nanosci.*, **1**, 259 (2004).

[5] K.J. Van Vliet, S. Suresh. Simulation of cyclic normal indentation of crystal surfaces using bubble raft model. *Philos. Mag. A*, **82**, 1993 (2002).

[6] K.J. Van Vliet, J. Li, T. Zhu, S. Yip, S. Suresh. Quantifying the early stages of plasticity through nano-scale experiments and simulations. *Phys. Rev. B*, **67**, 104104 (2003).

[7] G. Das, S. Ghosh, S. Ghosh, R.N. Ghosh. Material characterization and classification on the basis of material pile-up surrounding the indentation. *Mater. Sci. Eng. A*, **408**, 158 (2005).

[8] D.F. Bahr, W.W. Gerberich. Plastic zone and pileup around large indentations. *Metallurgical and Materials Transactions A—Physical Metallurgy and Materials Science*, **27**, 3793 (1996).

[9] A. Gouldstone, H.-J. Koh, K.-Y. Zeng, A.E. Giannakopoulos, S. Suresh. Discrete and continuous deformation during nanoindentation of thin films. *Acta Mater.*, **48**, 2277 (2000).

[10] Z.-H. Xu, J. Ågren. An analysis of piling-up or sinking-in behavior of elastic–plastic material under a sharp indentation. *Philos. Mag.*, **84**, 2367 (2004).

[11] R. Philips. *Crystals, Defects and Microstructures-Modeling Across Scales*, p. 206, Cambridge University Press, Cambridge (2001).