# COLLECTIVE PRISMATIC DISLOCATION LOOPS MECHANISM

Yoji Shibutani*, Tomohito Tsuru*
*Osaka University, Department of Mechanical Engineering & Systems, 565-0871 Suita, Japan

*Summary* Unstable displacement burst observed in the indent load and depth curve of nanoindentation is much possible to be related to the collective dislocation behavior. We have recently reported [1] that the first critical indent load at the first burst is almost linear to the first burst width. To resolve the reason of this experimentally obtained linearity, we must understand the collective prismatic dislocation loops mechanism. In the present research, the dislocation emission and the subsequent prismatic dislocation loop formation of a single crystalline aluminum under nanoindentation are simulated by the molecular dynamics. Also, the collective prismatic loops emitted due to the internal pressure by a rigid sphere embedded into the Al matrix are studied, qualitatively and quantitatively comparing with the micromechanics considerations.

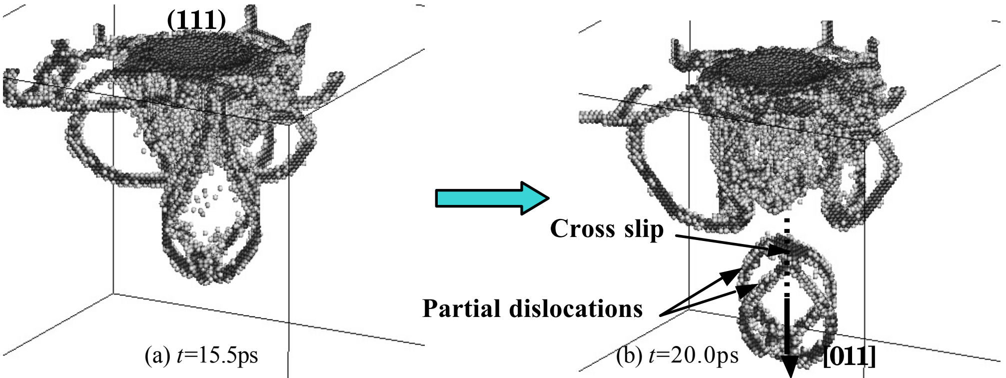
## INTRODUCTION

Indentation technique has been put to a wide use in order to obtain the hardness and the elastic properties of materials even at the nanoscale. Recently, it is worthy of notice that indent load and depth curves provide an opportunity to investigate the early events of plasticity (nano-plasticity). The distinctive displacement burst of indent depth observed in nanoindentation [2] is thought to be linked to the dislocation emission, being caused when the maximum shear stress generated under the indenter is of the order of the theoretical shear strength. Moreover, the experimentally obtained linear relation on the burst phenomena has recently been reported [1]. It is a fact that the first critical indent load at the first burst is almost linear to the first burst width. To resolve the reason of this linearity, we must understand the collective prismatic dislocation loops mechanism. In the present research, dislocation emission and the subsequent prismatic dislocation loop formation of a single crystalline aluminum under nanoindentation are simulated by the molecular dynamics (MD). Also, the collective prismatic dislocation loops emitted due to the internal pressure by a rigid sphere embedded into the Al matrix are studied as a reference, because the stress field is more predictable than that of the indentation. On the mechanism of the prismatic dislocation loop, the simple model with the misfitting particle in a ductile matrix has been acknowledged from the micromechanics view point [3]. Therefore, the latter atomistic stress states are compared with the elastic solution, discussing the nucleation mechanism of the collective dislocation loops.

## PRISMATIC DISLOCATION LOOP

### Nucleation due to Indentation

A prismatic dislocation loop due to the indentation is assembled by the shear loops emitted from the surface and then the cross-slip mechanism. It penetrates on the side surface of the spatially limited atomic model, leaving the rhombic steps. An example of the formation of prismatic dislocation loop emitted from the (111) surface of Al under the spherical punch with 5nm radius using the Finnis-Sinclair type many body potential is depicted in Fig.1.



(a) $t$=15.5ps (b) $t$=20.0ps

*Figure 1.* Formation of prismatic dislocation loop due to the indentation.

### Nucleation due to internal pressure by a rigid sphere in Al matrix

Studies concerned to the formation of prismatic dislocation loops have been performed experimentally in the past about fifty years. Many of those remarked about the presence of a spherical or a non-spherical precipitate inside a given crystalline matrix. Several quantitative analyses for the spherical particle geometry and a few studies for the non-spherical geometry exist. The nucleation of a shear dislocation loop from the interface of a misfitting spherical particle in a deformable matrix has been discussed in the Ref. [3], as shown in Fig.2. An initial shear loop emits on the slip plane at the maximum shearing stress at $z = a/\sqrt{2}$, where $a$ is radius of the particle ((a) in Fig.2). The screw segments on both sides of that dislocation move to each highly stressed cross-slip plane that is parallel to each other ((b) and (c) in Fig.2). Finally, the dislocation loop on the cross-slip plane moves to the next cross-slip plane that is parallel to the initial slip plane ((d) in Fig.2).

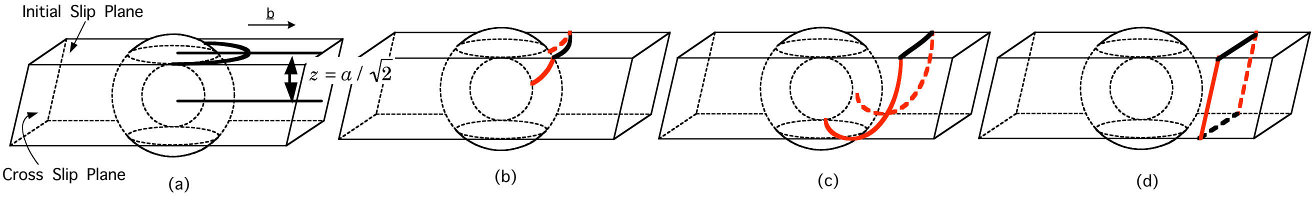


*Figure 2.* Formation of prismatic dislocation loop at a misfitting particle in ductile matrix [3].

The corresponding stress field to Fig.2 is atomistically realized in the MD simulations, as shown in Fig.3. Due to the increment of the internal pressure by the rigid sphere embedded into the Al matrix, a few shear loops are emitted at the interface whose the critical shear stress is 2.51GPa, one third of the critical pressure and one thirteenth of the shear modulus. Four different shear loops are simultaneously emitted from the same position ($z = a/\sqrt{2}$) from the center on the different family of slip planes $\{111\}$. And then they form a prismatic loop under the high-energy reactions between two shear loops.

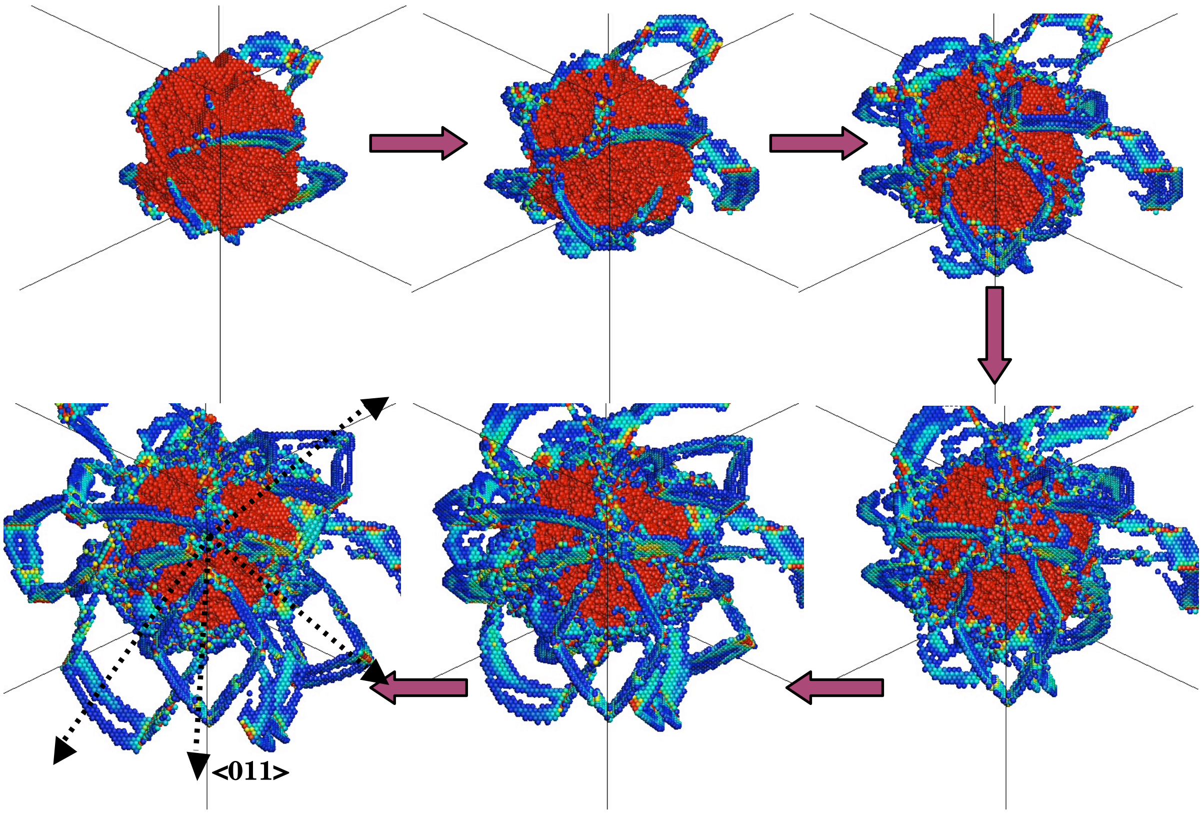


*Figure 3.* Formation process of the collective prismatic dislocation loops due to internal pressure in the Al matrix.

## CONCLUSIONS

We discussed the dislocation emission and the subsequent formation of the prismatic dislocation loop under nanoindentation and also due to the internal pressure in Al matrix by the molecular dynamics simulations. The latter atomic level stress states are in good agreement with the elastic solution and the collective mechanism was discussed.

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### References

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