

## INTERACTION BETWEEN DISLOCATION AND COHERENT TWIN BOUNDARY BY QUASICONTINUUM MODEL

TRAN H-S.<sup>1</sup>, TUMMALA H.<sup>2</sup>, DUCHÊNE L.<sup>1</sup>, PÉRON-LÜHRS V.<sup>1</sup>, FIVEL M.<sup>2</sup>,  
HABRAKEN A. M.<sup>1,3</sup>

<sup>1</sup>Dpt ArGEnCo, MS<sup>2</sup>F- MSM, University of Liège Chemin des Chevreuils 1, 4000 Liège, Belgium  
E-mail: hstran@ulg.ac.be; l.duchene@ulg.ac.be; vincent.peron@siemens.com;  
anne.habraken@ulg.ac.be  
[http://www.facsu.ulg.ac.be/cms/c\\_683942/en/materials-and-solid-mechanics-msm](http://www.facsu.ulg.ac.be/cms/c_683942/en/materials-and-solid-mechanics-msm)

<sup>2</sup> SIMaP-GPM2 INP Grenoble 101 Rue de la Physique BP46 38402 St Martin d'Herès cedex  
E-mail : Hareesh.Tummala@simap.grenoble-inp.fr; Marc.Fivel@grenoble-inp.fr  
<http://www.numodis.com>

<sup>3</sup>[F.R.S. FNRS](http://www.fnrns.be/) Fund for Scientific Research – FNRS  
<http://www.fnrns.be/>

**Key words:** Twin boundary, Dislocation, Nano-mechanics, Quasi-Continuum method

**Abstract.** The interaction between lattice dislocations and Coherent Twin Boundary  $\Sigma 3$   $\{111\}$  of copper has been studied using Quasi-Continuum method. The coherent twin boundary provides high barrier to slip transmission. The dislocation pile-up modifies the stress field at its intersection with the grain boundary. A different reaction process compared with the case of single dislocations is noticed. One observes the nucleation of a Lomer-type dislocation with Burgers vector of  $\frac{1}{2} \langle 110 \rangle$  and its glide on the (100) cube plane in the adjacent grain. This phenomenon has been observed with Transmission Electron Microscopy at room temperature and in other Molecular Dynamics simulations. We also show a novel interaction mechanism between Lomer-type dislocation and Coherent Twin Boundary. This interaction process leaves a dislocation with a Burgers vector coincident with the complete lattice shift of the Coherent Twin Boundary. Quantitative estimation of critical stress for various transmission phenomena is performed by using virial stress. Such information can be used as input for Discrete Dislocation Dynamics models

### 1 INTRODUCTION

In nanocrystalline (NC) metals which have a large grain boundary density, various mechanical properties depend on the interactions between dislocations and grain boundaries. Grain boundaries are effective sources, sinks and barriers for dislocations but many details of these interactions are not yet understood.

In FCC metals, conventional dislocations form and slip on  $\{111\}$  planes, however P. Karnthaler and Korner [1;2] observed the generation of Lomer dislocation  $a/2 \langle 110 \rangle$  glide on cube plane  $\{100\}$  under the influence of internal stress in low stacking-fault energy alloy by TEM studies. The glide of dislocations in unusual non-octahedral planes ( $\{110\}$ ,  $\{112\}$ ) was

also studied in [3]. Lee et al. showed the effect of Lomer dislocations as the source of strain hardening effect in nanotwinned metals [4]. Molecular Dynamics simulations have also confirmed the presence of Lomer dislocation slip [5-11].

The Coherent Twin Boundaries (CTBs) are of special interest because they have lowest energy and highest energy barrier for dislocation-GB interaction [7-9]. CTBs play a crucial role in the deformation behaviour of NC metals. Their study is of fundamental interest to identify atomistic mechanisms by which twin boundaries lead to strain hardening and to determine the resolved shear stress associated to slip transfer across CTBs.

The purpose of this paper is the use of Quasi-Continuum Method (QCM) to study the nucleation of Lomer dislocation and examine the effect of Lomer dislocation interacting with CTB at the atomistic scale. Taking copper as the prototype of FCC metals, we observed the generation of a  $a/2[110] \{001\}$  Lomer dislocation from the interaction of a  $90^\circ$  partial dislocation and a CTB. We also revealed a novel deformation mechanism in which a Lomer type dislocation interacts with the CTB to generate a Shockley partial dislocation and a step during the slip transfer reaction.

## 2 METHODS AND MODEL SET-UP

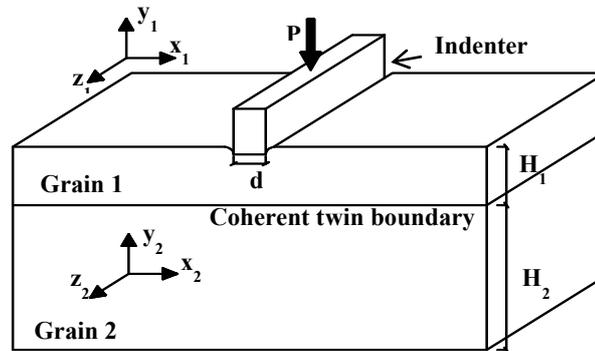
In this paper, we apply the Quasi-Continuum Method (QCM) developed by Tadmor and co-workers [12-14] to study the nucleation of Lomer dislocation and the interaction between dislocation and CTB coherent twin boundary in copper. The QCM is a molecular static technique finding the solution of equilibrium atomic configurations by energy minimization, for external loads or displacements. The problem is modeled without explicitly representing all the atoms in the cell; here the regions of small deformation gradients are treated as a continuum media by the finite element method.

The nanoindentation loading [15] is used as a “dislocation source”, in order to generate dislocations and probe the interaction of dislocations with the grain boundary. The simulation was carried out at a temperature of 0K using the Foils-Baskes-Daw embedded atom method (EAM) for copper [16]. The lattice constant is  $a_0 = 3.615 \text{ \AA}$ . The elastic parameters  $C_{11}$ ,  $C_{12}$ ,  $C_{44}$  are 110.9, 82.3, and 50.7 GPa, respectively. As shown in Figure 1, the studied computational domain of a bi-crystal model has an overall size of  $1000 \times 700 \text{ \AA}$  and contains one  $\Sigma 3 \{1 1 1\}$  CTB taken as the horizontal plane of the simulation box. Inside the domain near grain boundary and under the indenter, full atomistic (non-local) zones are provided. Outside the full atomistic zone, mesh coarsening is defined using a Delaunay triangulation over a set of nodes. The key advantage of QC code is the automatic adaptation [13] to ensure full atomistic resolution when dislocations are emitted as well as at the interactions between the dislocations and the grain boundaries. The thickness in  $Z$  direction is the minimum periodic distance for the crystalline orientation. The analysis is carried out in a 2D coordinate system, out-of-plane displacements are not allowed. Within this setting configuration only dislocations with line directions perpendicular to the plane of analysis can be nucleated and no variation in the out-of-plane  $z$ -direction can be sustained [12].

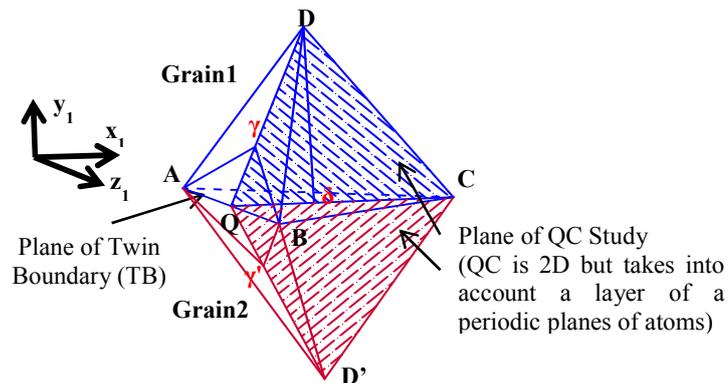
In our simulation, the orientations of grain 1 along  $X$  and  $Y$  directions coincide with  $[-1 -1 2]$  and  $[1 1 1]$  crystallographic directions, respectively. The CTB is produced by rotating of an angle of  $70.5^\circ$  around  $Z - [1 -1 0]$  axis a part of grain 1 which becomes grain 2. The distance  $H_1$  between the top surface of grain 1 and the CTB along the vertical direction  $Y$  is  $H_1=200 \text{ \AA}$ .

Note that other  $H_1$  values were tested, however shorter values prevent an easy differentiation of the mechanisms when higher ones produced similar observations with longer CPU time.

The indenter is a rigid rectangular block. The number of atoms in contact with it remains constant and a displacement boundary condition is applied to these atoms. The indenter size is fixed at a width of  $60 \text{ \AA}$  ( $d$  value in **Figure 1**) in order to limit the mutual interaction between the two generated systems of a dislocation dipole. The boundary condition of the surface aside from the indenter zone is left free. The volume of simulation was chosen to ensure that far-field boundary conditions did not affect the relaxed configuration of the CTB and the behavior in the vicinity of the indenter. The system investigated here would have been quite large for a standard full atomistic simulation. However using QCM greatly reduces the number of degrees of freedom (only 10000 atoms are explicitly treated at the end of the simulation). An incremental displacement of atoms located under the indenter is applied per step and the equilibrium of system is found by minimizing the energy. At each step, the minimum of the energy is found using a conjugate gradient method. Atoms belonging to a defect (grain boundary or dislocation core) are distinguished based on the Centro Symmetric Deviation parameter [17]. In order to evaluate mechanical properties at the atomic scale, the virial stress which is equivalent to the mechanical Cauchy stress [18] is calculated without the kinetic portion as the simulation assumes a constant temperature of 0 K.



**Figure 1:** Schematic representation of the nanoindentation model of a bicrystal in with a CTB



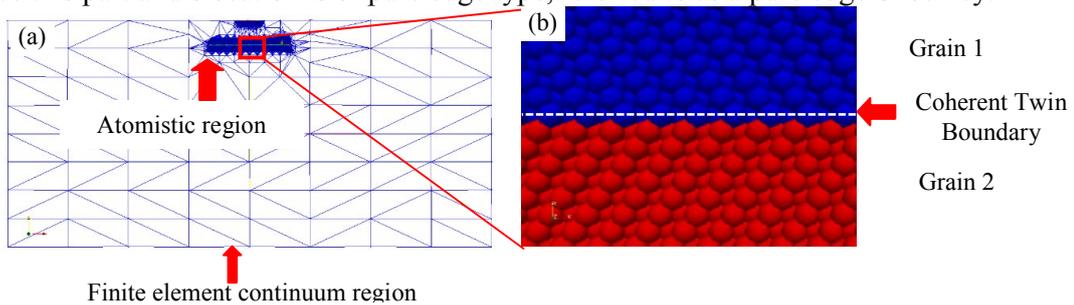
**Figure 2:** The double Thompson's tetrahedron for the consistent twin boundary and the matrix orientation relationship. The Coherent- Twin Boundary plane is defined as the (1 1 1) ABC plane

### 3 ANALYSIS OF QC RESULTS

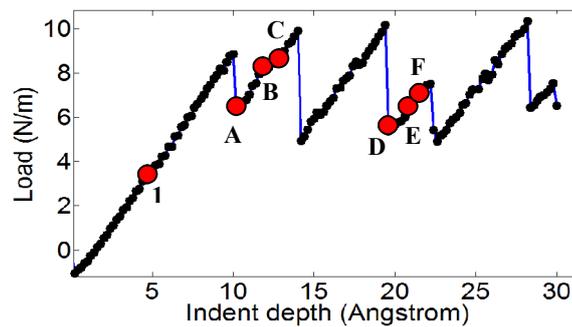
The simulation describes the nucleation of dislocations beneath the indenter vs imposed displacement. Analyzing the Centro Symmetric Deviation (CSD) parameter dislocation structure, the interactions between partial dislocation and Lomer dislocation with CTB are observed. In addition, the atomic stress field evolution is obtained by QCM.

#### 3.1 Loading vs. indent depth and dislocation emission

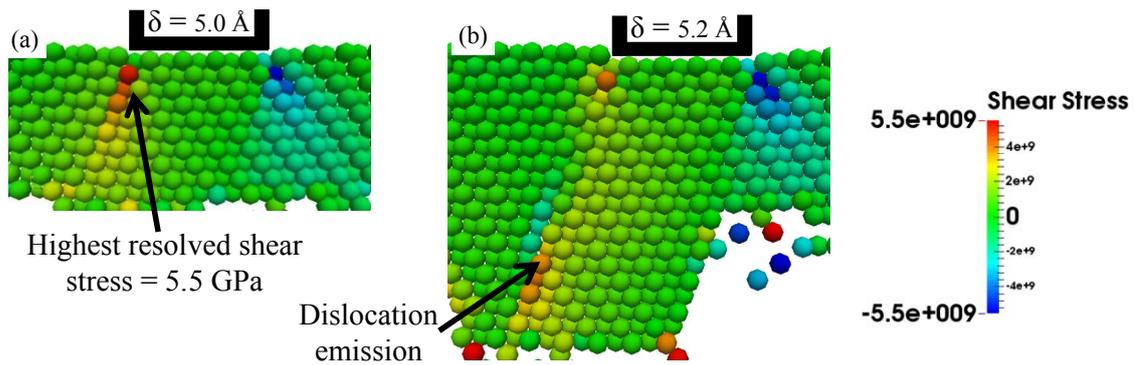
Figure 3 shows the entire QC model and the relaxed atomistic configuration of the CTB is presented in the zoom zone. The loading displacement step of indenter  $\Delta\delta$  is 0.2 Å. Note that a smaller loading step of 0.1 Å was also used and provided identical results. **Figure 4** displays the computed curve linking the loading force and the indent depth  $\delta$ . This load-displacement curve begins with a linear relation and a first drop at 10 Å. The strong decrease does not correspond to the nucleation of the first dislocation beneath the indenter. The first dislocation is nucleated at indent depth  $\delta = 5$  Å (Point 1 in **Figure 4**). When the local shear stress reaches 5.5 GPa (**Figure 5-a**), the first partial dislocation nucleates (**Figure 5-b**). The computed nucleation stress value is in good agreement with estimation theory ( $G/2\pi$ ). A view of the atomic structure of this dislocation is shown in **Figure 6**. In order to analyze this dislocation, a Burgers circuit around the dislocation starting at S and ending at F was drawn in the (1 -1 0) plane, showing a closure failure from F to S. It allows identifying a partial dislocation of type  $D\gamma$  partial with Burgers vector  $b = 1/6 [1 1 2]$  with a  $[-1 -1 0]$  line direction in the (-1 -1 1) face of the Thompson tetrahedron (**Figure 2**). No out-of-plane displacement was generated since this partial dislocation is of pure edge type, referred to as a pure edge Shockley.



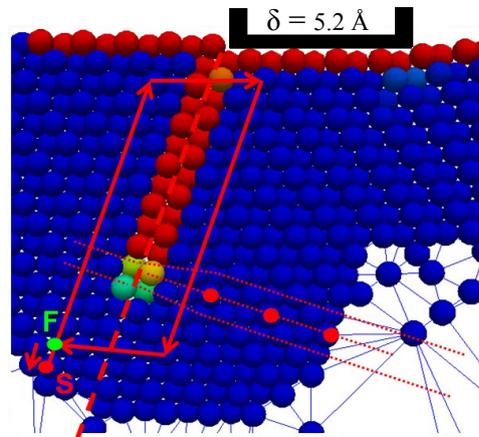
**Figure 3:** (a) Overview of the entire system with domain partition in full atomistic and finite element zones of a nanoindentation experiment, (b) atomistic configuration of CTB after relaxation



**Figure 4:** Load - Indent depth  $\delta$  curve for a nanoindentation test into a (111) face of a bi-crystal model presenting a CTB  $\Sigma 3 \{111\}$



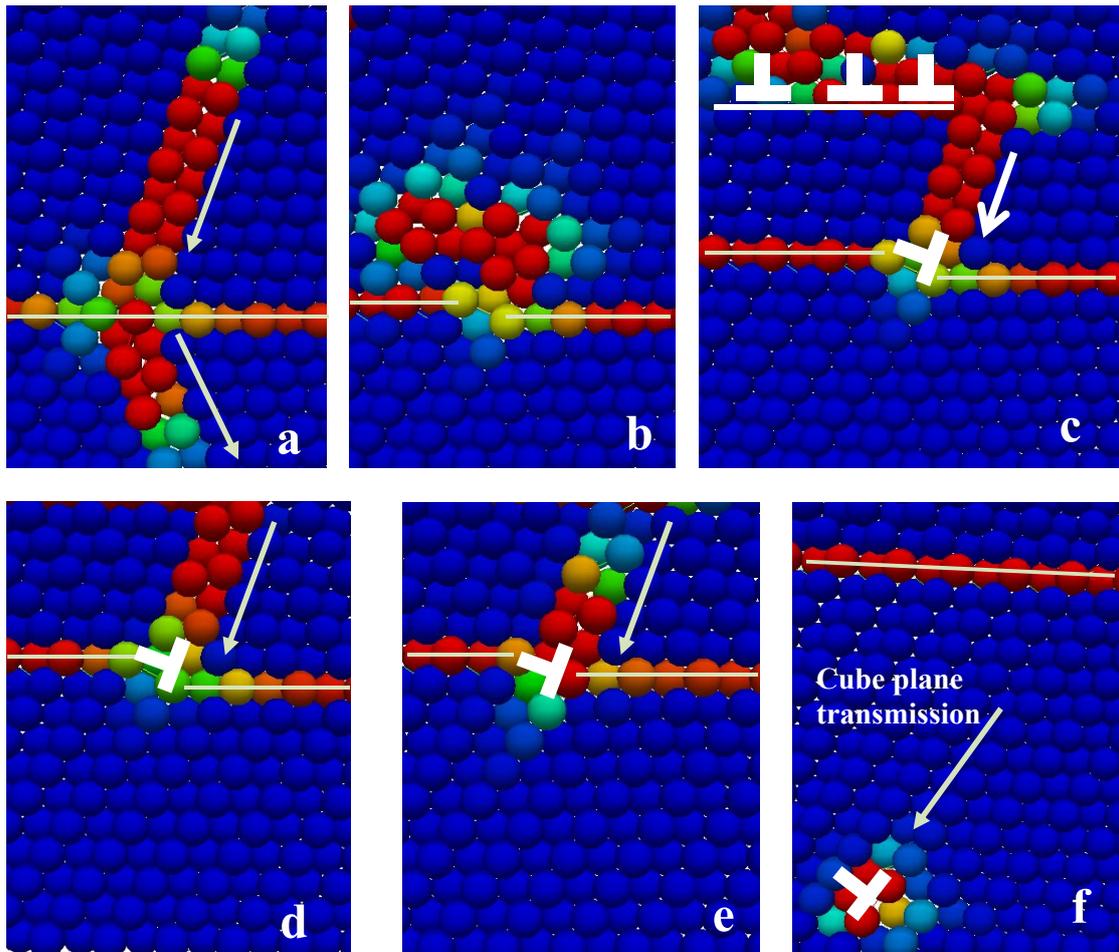
**Figure 5:** Atomic shear stress (Pa) beneath the indenter before (a) and after (b) nucleation of partial dislocation



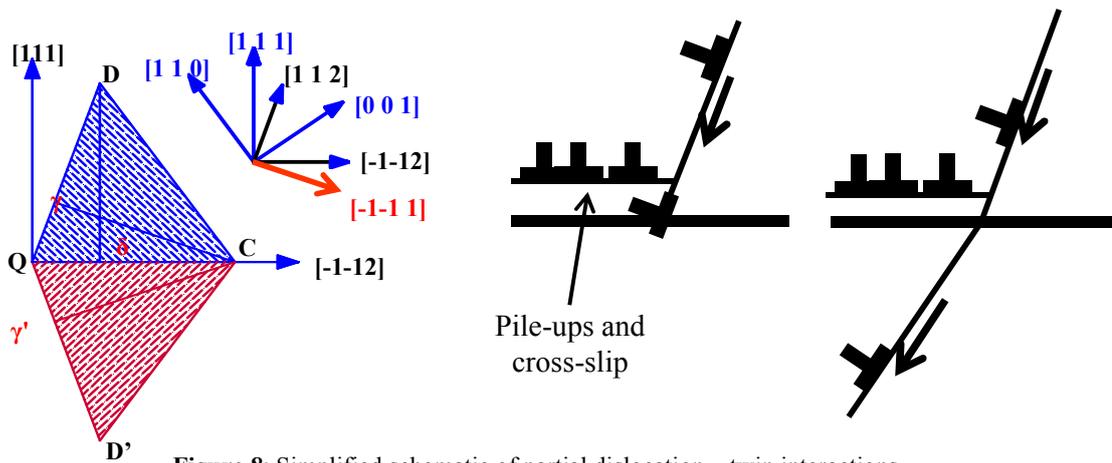
**Figure 6:** The atomistic structure visualized by CSD parameter of 90° partial dislocation (indent depth is 5.2 Å)

### 3.2 Partial dislocation/Twin Boundary interaction mechanism

As the deformation progresses, an additional partial dislocation is nucleated on the adjacent plane and this second 90° partial dislocation also moves toward the CTB. This later dislocation is blocked by the CTB at an accumulated indentation depth of 10 Å (**Figure 7 a**). We noted an incomplete transmission, this is partly because of low Schmid factor of this system in given loading direction and high stability and coherency of the twin boundary. In this process, a pile-up and cross-slip of dislocations at the intersection site are created (**Figure 7 b-c**). With increasing load, the high local stress forces the dislocation to transmit the GB on a non-Schmid, cubic {100} cube plane rather than gliding in the regular slip plane, thus nucleating a Lomer-type dislocation which glides in the adjacent grain. This is illustrated in **Figures 7 d-f**. This phenomenon has been observed by other scientists in experiments (at room temperature of low stacking fault FCC alloys) [1-3] and in MD simulations [5-11;19] [20]. Figure 8 presents a simplified schematic of the partial dislocation – twin interactions



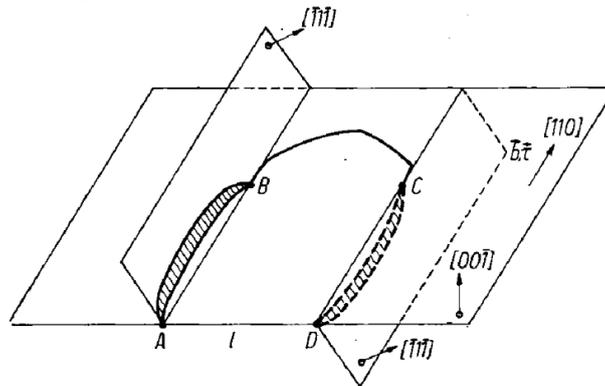
**Figure 7:** Snapshots of partial dislocations pile up (a-e) and the formation of a Lomer dislocation of Burgers vectors  $b = \frac{1}{2} \langle 110 \rangle$  on the  $\{100\}$  plane visualized by CSD parameter. The corresponding indent depths are 10.2 Å (a), 12.6 Å (b), 12.8 Å (c), 20.0 Å (d), 22.4 Å (e), 22.6 Å (f) respectively.



**Figure 8:** Simplified schematic of partial dislocation – twin interactions

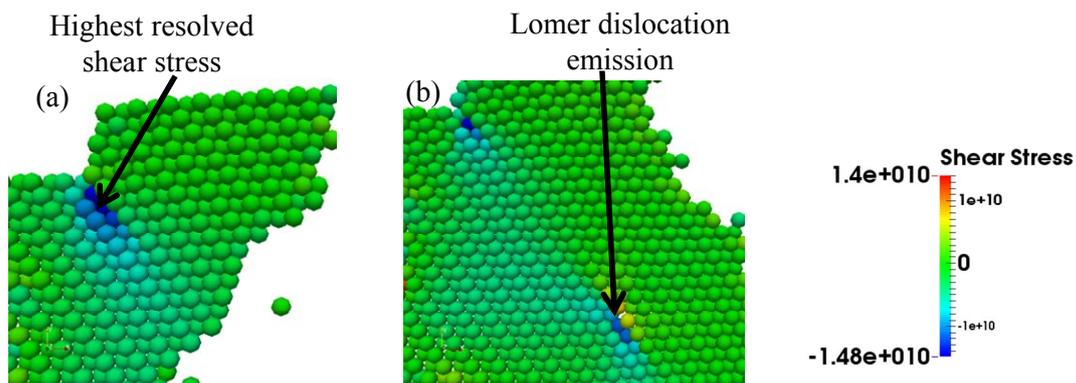
### 3.3 Lomer dislocation/Twin Boundary interaction mechanism

Korner *et al.* [2] showed that when parts of this half loop reach screw orientation, the total dislocation gliding on (001) can cross-slip onto a {111} plane and dissociate into Shockley partial dislocations thus reducing the global energy (**Figure 9**). In the case of Lomer type dislocation, only edge component glide on {100} planes. Therefore, we are only focused on the interaction between edge Lomer dislocation with another defect.

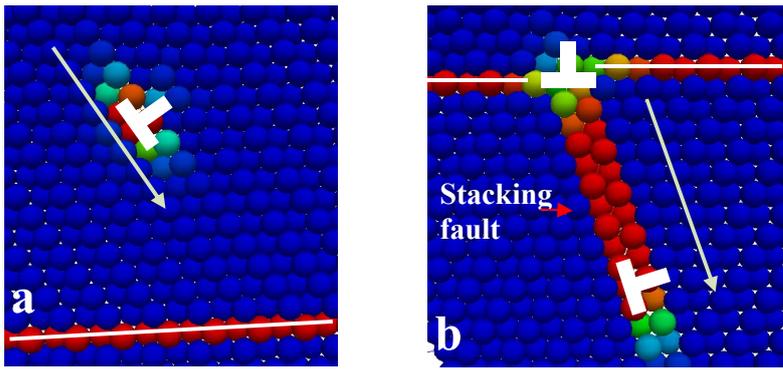


**Figure 9:** The screw components (AB and CD) have cross-slipped and dissociated into partials on {111} planes. The dislocation arm BC lies in the (001) plane. [2]

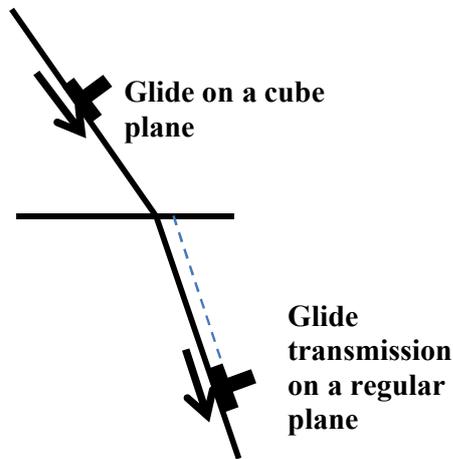
At an accumulated indentation depth of 18.0 Å, the local shear stress reaches 14.8GPa (Figure 10). One observes a Lomer dislocation type emitted from the corner of the indenter and it glides in the  $[-1 -1 0]$  direction on the (0 0 1) cube plane (**Figure 11 a**). The nucleation stress of the Lomer dislocation is three times higher than the usual ones reported in 3.1. This incident dislocation, once it has reacted with the CTB, nucleates a partial dislocation within the CTB and a step appears at the intersection (**Figure 11 b**). This Shockley partial dislocation has a Burgers vector  $b' = D'\gamma'$  in the  $A'B'D'$  face of the Thompson tetrahedron (**Figure 2**). The partial dislocation moves down and away from CTB laying down a stacking fault in its wake. **Figure 12** shows the schematic of Lomer dislocation – twin interaction. After transmission, the residual stress is observed at CTB (**Figure 13**).



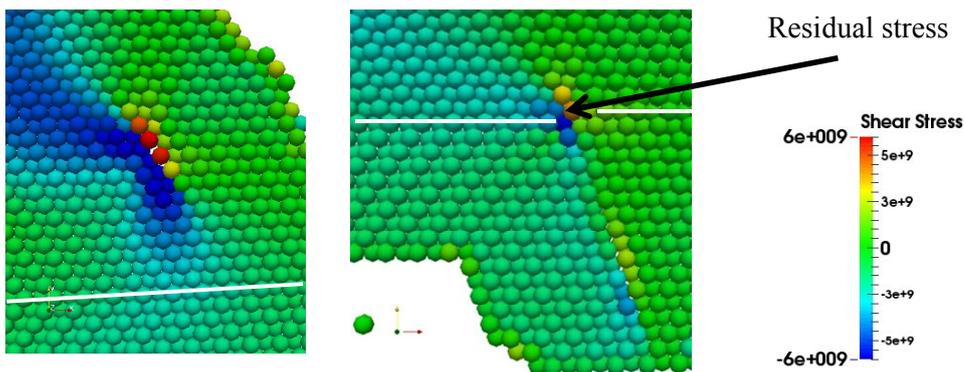
**Figure 10:** Atomic shear stress (Pa) beneath the indenter before (a) and after (b) the nucleation of a Lomer dislocation



**Figure 11:** Incident Lomer-dislocation interacts with CTB creating a glissile partial dislocation in the twinned region and a step at the intersection between initial dislocation and CTB (visualized by CSD parameter). The corresponding indent depths are 18.2 Å (a), 20.0 Å (b) respectively.



**Figure 12:** Simplified schematic of Lomer dislocation – twin interactions



**Figure 13:** Interaction process of an Lomer dislocation and CTB visualized by atomic shear stress (Pa) associated with the steps in Figure 11

#### 4 CONCLUSIONS

The present work extends our understanding of the nucleation and interaction between Lomer type dislocations and CTB. The results support the following conclusions:

- Under [111] compression loading, different interactions have been observed. The results show the details of the dislocation nucleation mechanism and the behavior of a Shockley partial and a Lomer type dislocation at the CTB.
- The Lomer-type dislocation is not common in FCC metals, therefore we might conclude that the potential proposed by Foiles-Baskes-Daw can predict the nucleation, the motion and the interaction mechanisms of this anomalous dislocation with other defects such as CTB. The critical yield stress for the nucleation of a Lomer dislocation has been quantified at about 14.8 GPa
- The QC simulations show that CTB is a strong barrier to slip transmission because of the discontinuity of slip systems. The transmission of a dislocation across a CTB can only take place at high applied stresses.
- Our results indicate that the complex mechanisms of interactions between dislocation and grain boundary might be analyzed using the Quasi-Continuum Method which can provide: Grain Boundary–Dislocation interaction mechanism analysis, estimation of critical stress for dislocation nucleation or transmission.

#### ACKNOWLEDGEMENTS

This research has been funded by the Interuniversity Attraction Pole Program initiated by the Belgian Science Policy Office, IAP7/21. AM Habraken thanks the F.R.S. FNRS which finances her work.

#### REFERENCE LIST

- [1] Karnthaler HP. The study of glide on {001} planes in f.c.c. metals deformed at room temperature. *Philosophical Magazine A* 1978 Aug 1;38(2):141-56.
- [2] Korner A, Karnthaler HP. Glide dislocations on cube planes in a low stacking-fault energy alloy. *phys stat sol (a)* 1983 Feb 16;75(2):525-35.
- [3] Caillard D, Martin JL. Glide of dislocations in non-octahedral planes of fcc metals: a review. *IJMR* 2009 Oct 1;100(10):1403-10.
- [4] Lee JH, Holland TB, Mukherjee AK, Zhang X, Wang H. Direct observation of Lomer-Cottrell Locks during strain hardening in nanocrystalline nickel by in situ TEM. *Sci Rep* 2013 Jan 14;3.
- [5] Wang J, Huang H. Novel deformation mechanism of twinned nanowires. *Applied physics letters* 2006;88(20):203112.

- [6] Marian J, Knap J, Ortiz M. Nanovoid Cavitation by Dislocation Emission in Aluminum. *Phys Rev Lett* 2004 Oct 14;93(16):165503.
- [7] Sangid MD, Ezaz T, Sehitoglu H, Robertson IM. Energy of slip transmission and nucleation at grain boundaries. *Acta Materialia* 2011 Jan;59(1):283-96.
- [8] Ezaz T, Sangid MD, Sehitoglu H. Energy barriers associated with slip–twin interactions. *Philosophical Magazine* 2011 Feb 2;91(10):1464-88.
- [9] Sangid MD, Ezaz T, Sehitoglu H. Energetics of residual dislocations associated with slip-twin and slip-GBs interactions. *Materials Science and Engineering: A* 2012 Apr 30;542(0):21-30.
- [10] Deng C, Sansoz F. Fundamental differences in the plasticity of periodically twinned nanowires in Au, Ag, Al, Cu, Pb and Ni. *Acta Materialia* 2009 Dec;57(20):6090-101.
- [11] Zhang X, Misra A, Wang H, Lima AL, Hundley MF, Hoagland RG. Effects of deposition parameters on residual stresses, hardness and electrical resistivity of nanoscale twinned 330 stainless steel thin films. *Journal of applied physics* 2005;97(9):094302.
- [12] Tadmor EB, Ortiz M, Phillips R. Quasicontinuum analysis of defects in solids. *Philosophical Magazine A* 1996 Jun 1;73(6):1529-63.
- [13] Shenoy VB, Miller R, Tadmor E, Rodney D, Phillips R, Ortiz M. An adaptive finite element approach to atomic-scale mechanics – the quasicontinuum method. *Journal of the Mechanics and Physics of Solids* 1999 Mar 1;47(3):611-42.
- [14] Miller R, Tadmor EB. The Quasicontinuum Method: Overview, applications and current directions. *Journal of Computer-Aided Materials Design* 2002;9(3):203-39.
- [15] Péron-Lührs V, Jérusalem A, Sansoz F, Stainier L, Noels L. A two-scale model predicting the mechanical behavior of nanocrystalline solids. *Journal of the Mechanics and Physics of Solids* 2013 Sep;61(9):1895-914.
- [16] Foiles SM, Baskes MI, Daw MS. Embedded-atom-method functions for the fcc metals Cu, Ag, Au, Ni, Pd, Pt, and their alloys. *Phys Rev B* 1986 Jun 15;33(12):7983-91.
- [17] Kelchner CL, Plimpton SJ, Hamilton JC. Dislocation nucleation and defect structure during surface indentation. *Phys Rev B* 1998 Nov 1;58(17):11085-8.
- [18] Subramaniyan AK, Sun CT. Continuum interpretation of virial stress in molecular simulations. *International Journal of Solids and Structures* 2008 Jul;45(14–15):4340-6.
- [19] Afanasyev KA, Sansoz F. Strengthening in Gold Nanopillars with Nanoscale Twins. *Nano Lett* 2007 Jul 1;7(7):2056-62.

- [20] Wu ZX, Zhang YW, Srolovitz DJ. Dislocation–twin interaction mechanisms for ultrahigh strength and ductility in nanotwinned metals. *Acta Materialia* 2009 Sep;57(15):4508-18.