

# MD ANALYSIS OF DISLOCATION NUCLEATION NEAR A FREE SURFACE

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Molecular dynamics analyses of aluminum single crystal strips subject to bending are carried out to investigate dislocation nucleation from free surfaces. The embedded atom method with the Ercolessi and Adams potential for aluminum is used. The strip has a rectangular cross-section in the plane of deformation while out of plane periodic boundary conditions are imposed so that the depth of the strip is effectively infinite. Loading is imposed through prescribed displacements that correspond to a pure rotation of the sides of the strip. The normal to the plane of deformation is the  $[111]$  direction and the loading is imposed on a plane normal to the  $[\bar{1}01]$  direction. Two types of free surfaces are analyzed: perfect surfaces and surfaces with atomic level step defects. The character of the dislocations nucleated is identified. The characterization of dislocation nucleation in terms of various potential nucleation criteria is explored. We find that:

- The initial dislocation structure consists of half-loops that are nucleated simultaneously on  $\{111\}$  planes for perfect free surfaces, while dislocations in  $\{111\}$  planes with  $\langle 110 \rangle$  directions are nucleated for stepped surfaces. The size of the incipient half-loops is approximately one seventh of the strip height.
- For perfect surfaces, dislocations nucleate only from the compressive side of the bent strip. On the other hand, when step defects are present dislocation nucleation can take place from either the compressive side or the tensile side.
- Values of the slip system resolved shear stress at nucleation are much lower than reported for dislocation nucleation in the bulk.
- Dislocation nucleation is not well-characterized by a critical value of the slip system resolved shear stress.