

Mechanical Strengthening in Gold Thin Films: A Molecular Dynamics Analysis of Nanoindentation Effects

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INTRODUCTION & AIM

As nanotechnology continues to progress, nano-scale thin films are seeing growing applications in various fields, including high-density storage systems, magnetic media, and micro/nanoelectromechanical systems (MEMS/NEMS). Nevertheless, in numerous thin film applications, the overall performance is often compromised by mechanical weaknesses encountered during practical use. Recently, Gold (Au) plays a pivotal role as a crucial material, thanks to its exceptional qualities most notably, its remarkably high electrical conductivity and impressive ductility. Its outstanding conductivity is indispensable in key technological applications like electronics and telecommunications. Moreover, the metal's notable ductility allows it to be fashioned into slender wires or intricate shapes, expanding its versatility across a wide range of manufacturing processes in different industries. Consequently, exploring the mechanical properties of thin films becomes imperative for assessing and enhancing their reliability. This research focused on the effects of different penetration velocities, extending our exploration of nanoindentation deformation mechanisms. The results of this study further our understanding of the complex processes that occur at the nanoscale during indentation. By systematically varying the velocities of the indenters, we reveal insights into the responses of the materials that can enrich our understanding of mechanical behavior at this scale. This insight not only contributes to fundamental scientific knowledge but also holds promise for practical applications, influencing the refinement and optimization of nanoindentation techniques. Ultimately, this research provides a valuable starting point towards improving our ability to manipulate and characterize nanoscale materials with greater precision and reliability.

METHOD

In Fig.1, we show the 3D schematic model of an Au thin film with a lattice constant of 4.08 Å. The dimensions of the Au film were 7.5 nm x 4.5 nm x 7.5 nm containing a total of 14,900 atoms with the crystallographic directions of [100], [010] and [001] in the X, Y, and Z axes, respectively. As shown in Fig.1, the Au film was categorized into three distinct atomic layers: bottom, middle, and upper layers. The lowermost three layers were established as rigid supports to diminish boundary effects and maintain the film's stability during the indentation process. The subsequent five layers in the middle were designated as thermostatic atoms, strategically crafted to enhance heat conduction within both the film and the indenter. Meanwhile, the atoms within the uppermost 14 layers are unrestricted in their movement, adhering to the principles of Newtonian equations. The constructed atomic configuration was allowed to relax for an appropriate duration under the NVT ensemble by using the Nosé-Hoover thermostat. In this simulation, a spherical indenter with a radius of 3 nm was positioned above the Au film at a distance of 0.5 nm. During the indentation process, the indenter moved at various velocities (5, 10, and 15 m/s) toward the surface of the Au film, penetrating it until reaching an indentation depth of 10 Å. In this study, all MD simulations were performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software.

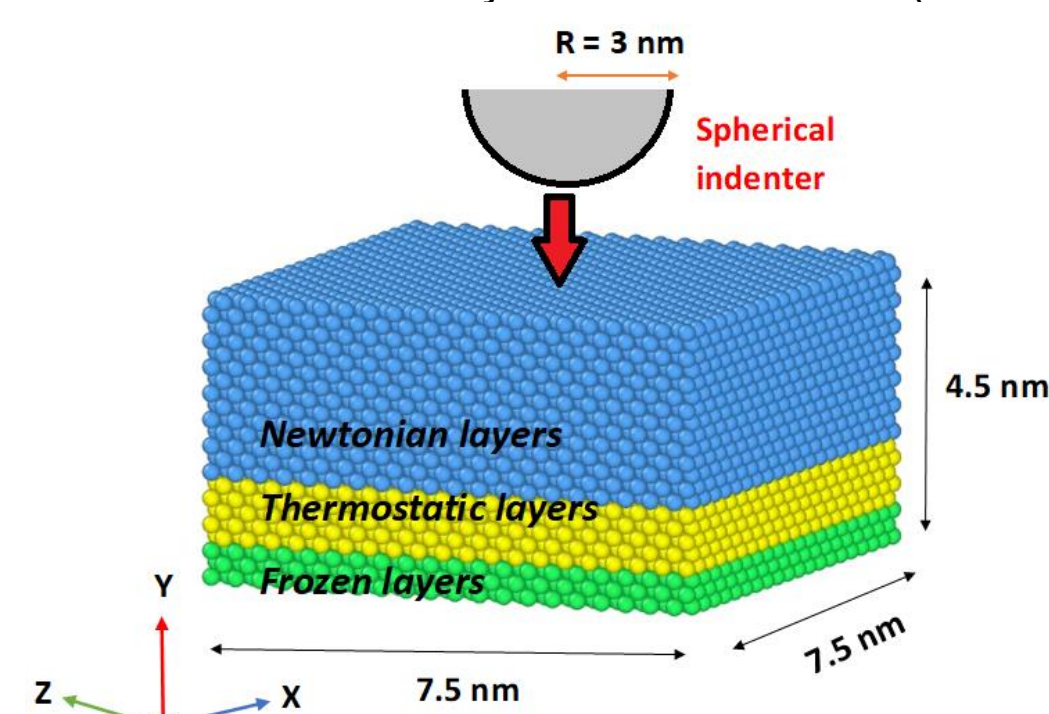


Fig 1:3D configuration model of Au film.

The study aims to understand the intricate deformation processes of an Au film during nano-indentation by deliberately varying indenter velocities (ranging from 5 m/s to 15 m/s). This intentional variation serves as a crucial parameter, allowing a systematic exploration of how different indenter speeds impact atomic rearrangements within the pivotal contact region between the indenter tip and the film surface. The insights derived from the experiment provide valuable data for refining and optimizing nano-indentation techniques, offering a pathway to precisely manipulate and control material properties at the atomic level. Consequently, the study contributes not only to understanding the specific behavior of the Au film but also to the broader field of nanoscale material manipulation and characterization. It is important to explore the impact of indentation velocity on the deformation mechanisms and properties of thin films. In Fig.2, we show the deformation region of the Au surface when performing nanoindentation (left part), and (the right part) displays the contour of the corresponding Au surface profile at different velocities. From these figures, it is evident that the pile-up shape was formed due to the force applied by the spherical indenter during the indentation process. The results reveal that the indented Au surface was affected by varying indentation velocities. In Fig.2 a2, the indented region has approximately smaller displacement due to the lower velocity of 5 m/s. This behavior was reported in the investigation of metallic materials. In contrast, as indentation velocities increase to 10 and 15 m/s (see Fig.2 b2, c2), the deformation shape shows a higher displacement of atoms. This observation suggests that the atoms in the indented region of Au are spread to a deeper displacement, which causes plastic deformation.

RESULTS & DISCUSSION

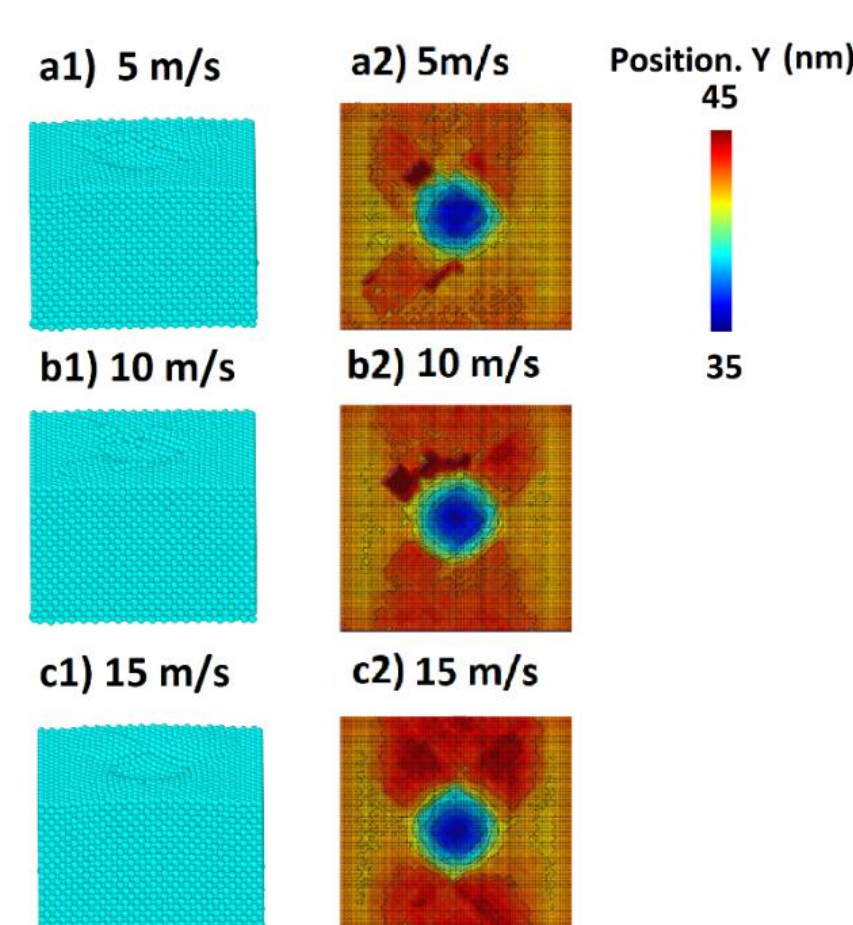


Fig 2:Indentation process of Au film surface.

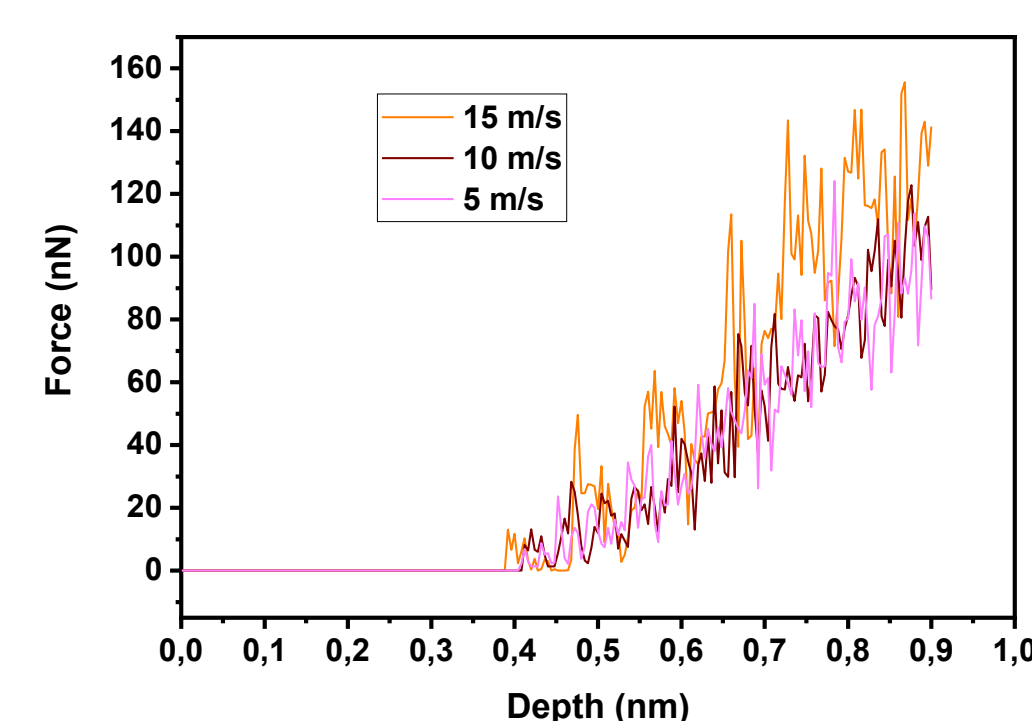


Fig 3: Load as a function of various velocity.

Fig.3 shows the resulting force-depth curve during the indentation process. It is evident that the force increases as the indentation depth increases. At a low velocity of 5 m/s, a smoother force-depth curve was observed. However, as the velocity increases, more pronounced serrations appeared and became more pronounced at an indentation velocity of 15 m/s. The existence of serrations in the indented Ag film can be attributed to atomic rearrangement and stacking faults. At higher velocities, the indentation process undergoes swifter and more dynamic loading. Consequently, a greater number of forces are exerted on the Au film, leading to a disturbance in the normal arrangement of atoms within the crystal lattice. As a result, this may heighten the likelihood of dislocation nucleation, leading to concurrent plastic deformation in the film [19].

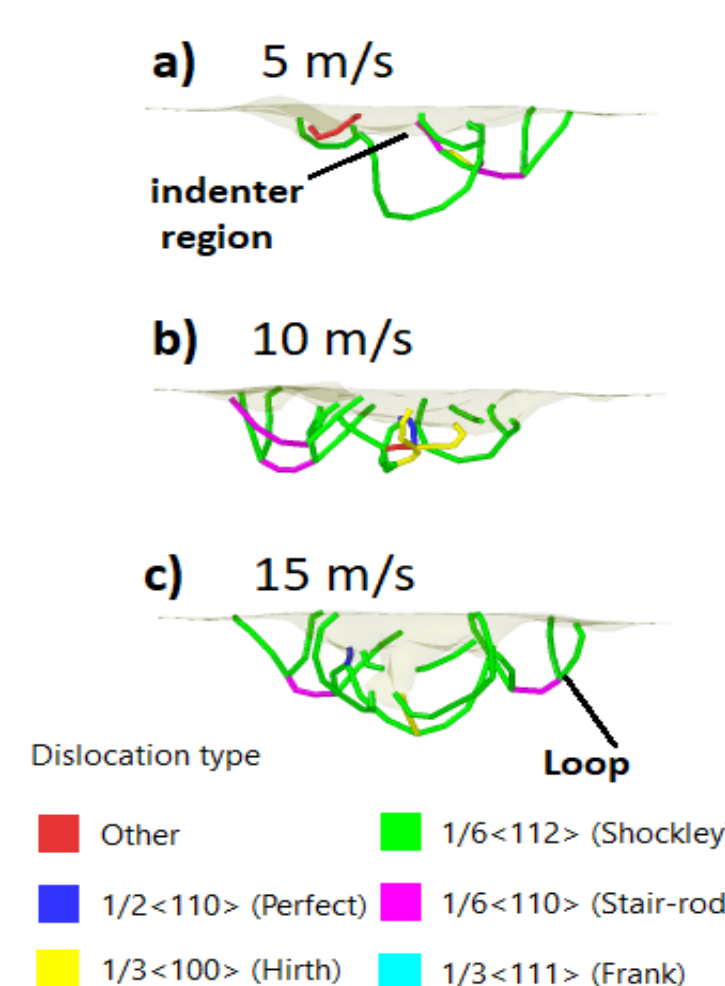


Fig 4:DXA analysis of Au thin film.

In Fig.4, we show the obtained analysis of dislocation formation within the Au film. The results clearly demonstrate the nucleation of dislocations along the (111) plane at various indentation velocities. In all instances, diverse types of dislocations were identified, including Perfect, Shockley, Stair-rod, and Hirth. These observations align with findings reported at different indenter velocities. In Fig. 4 c, it is apparent that a dislocation loop has formed within the Au film, with a full dislocation branching out to create two Shockley and Stair-rod partial dislocations, indicated by the circular shape. However, as the indentation velocity increases to 15 m/s, the dislocation density intensifies, accumulating around the indenter region. The emergence of this dislocation type may arise from the movement of Shockley partial dislocations within distinct {111} crystallographic planes, where they interact along the <110> direction. In all cases, it is evident that the Shockley partial dislocations are considered dominant partial dislocations. Such behavior could play a role in causing strain hardening in the indenter film. This occurrence is attributed to the fact that accumulated dislocations, with escalating velocities, impede each other's motion, making it more challenging for them to traverse the crystal lattice. This phenomenon contributes to enhancing the hardness properties of the film.

CONCLUSION

This research focuses on the nanoindentation of gold (Au) materials to enhance our understanding of their deformation responses and mechanical properties. Utilizing the Molecular Dynamics (MD) method, we simulated the impact of indentation velocity on nanoindentation force-depth, hardness, and dislocation mechanisms. As the indentation velocity increased to 15 m/s, we observed the initiation of dislocation propagation and nucleation. Moreover, the determination of hardness in Au displays a notable reliance on the indentation velocity. The lowest hardness is observed at a low indentation velocity of 5 m/s, while the highest value is attained at 15 m/s. The DXA analysis reveals that a reduced number of dislocations is generated at an indentation velocity of 5 m/s. In contrast, an elevated quantity of dislocations becomes apparent as the indentation velocity is extended to 15 m/s. These findings suggest a heightened hardness in the specimen, particularly notable as the indentation velocity becomes greater.

FUTURE WORK / REFERENCES

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