THERMO-MECHANICAL PROPERTIES OF 2D MONOLAYER GOLD: A MOLECULAR DYNAMICS STUDY

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I. INTRODUCTION

- 2D materials have unique thermal and mechanical properties.
- Gold can form a stable monolayer with a triangular lattice.
- This study simulates its thermal stability and mechanical deformation using LAMMPS and EAM potential.

II. SIMULATION METHODS

- Potential: EAM (Au_u3.eam)
- Model: ~1000 atoms, triangular lattice
- BCs: Periodic (x, y), vacuum (z)
- Thermal test: NPT, 300–2000 K
- Mechanical test: NVT, tension x & y
- Strain rate: 0.001 ps^{-1}, timestep: 0.001 ps

III. RESULTS AND DISCUSSION

3.1 Structural Relaxation and Geometry

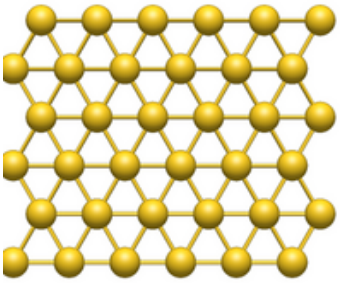

Figure 1. *Atomic-scale view of the triangular lattice structure in the gold monolayer.*

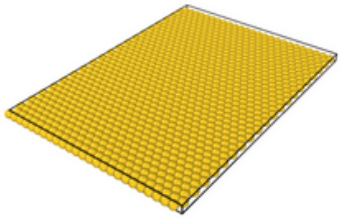

Figure 2. *Side view of the relaxed gold monolayer structure.*

Relaxed structure has bond length ≈ 2.66782 Å

3.2 Thermal Stability and Phase Transition

- Energy and volume increase rapidly in the range of 1500–1600 K, suggesting a phase transition.
- The specific heat capacity (Cp) shows a sharp peak at ~1593 K, indicating the transition temperature.

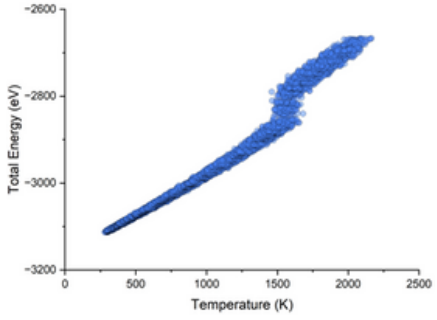

Figure 3. *Total energy as a function of temperature.*

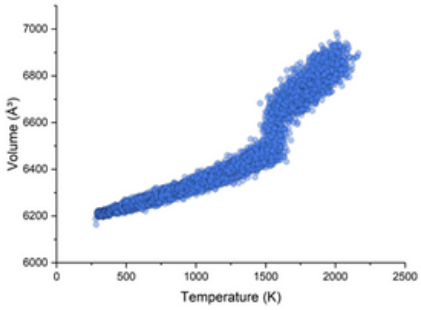

Figure 4. *Volume expansion behavior with temperature.*

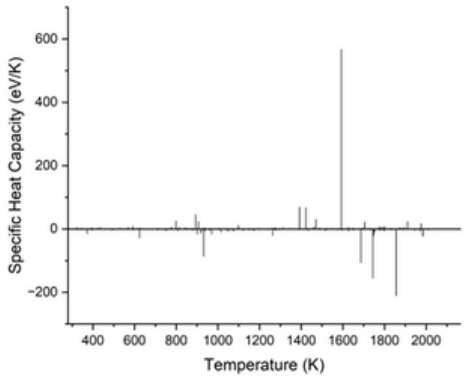

Figure 5. *Specific heat capacity curve derived from energy–temperature data.*

3.3 Stress–Strain Analysis

- Fracture strain: 10.99% (x), 9.14% (y)
- Max stress: 41.25 GPa (x), 38.36 GPa (y)
- Young's modulus nearly equal in x/y → elastic isotropy

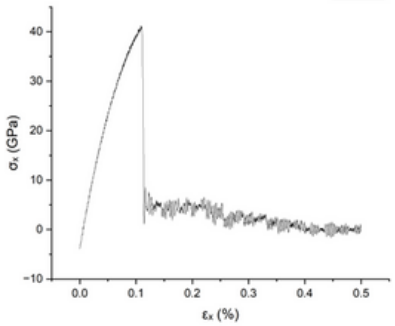

Figure 6. Stress–strain behavior under uniaxial tension along the x-direction at 300 K.

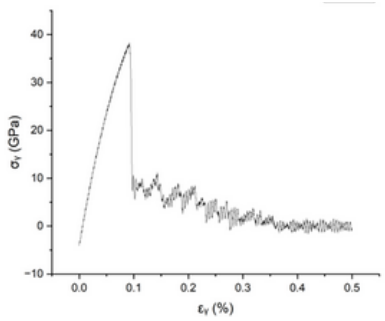

Figure 7. Stress–strain behavior under uniaxial tensile loading along the y-direction at 300K.

IV. CONCLUSIONS

- 2D gold is stable up to 1500 K
- Exhibits phase transition near 1593 K
- Slight anisotropy in fracture but isotropic in elasticity
- Promising for flexible electronics and thermal sensors