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SIMULATION DRIVEN METHODOLOGY TO GENERATE AND OPTIMIZE COPPER NANOSHEETS

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Abstract

The advancement of nanoscale material science relies heavily on accurate computational methodologies capable of capturing the structural and energetic behavior of metallic nanostructures. In this study, we present a simulation-driven framework for generating and optimizing two-dimensional copper nanosheets using the Gupta potential, a semi-empirical many-body potential tailored for transition metals. The methodology begins with constructing atomic configurations based on the face-centered cubic (FCC) lattice, followed by relaxation and optimization processes that account for realistic interatomic interactions and surface effects. This approach enables systematic generation of nanosheets with tunable crystallographic orientations, thicknesses, and edge terminations. The resulting structures exhibit physically consistent geometries and energetics aligned with available experimental observations. Our findings demonstrate the efficiency and reliability of this computational technique, offering a robust platform for exploring the mechanical, electronic, and catalytic properties of copper nanosheets. The methodology also establishes a foundation for extending simulations to other metallic systems using the Gupta potential framework.

1. INTRODUCTION

Two-dimensional nanostructured materials have attracted significant interest due to their high surface-to-volume ratios and unique physicochemical properties. Among these materials, copper nanosheets (Cu NSs) represent a promising class of two-dimensional metallic systems with applications spanning catalysis, nanoelectronics, transparent conductive films, plasmonics, and energy storage [1-3]. Their excellent thermal stability, high electrical conductivity, and cost-effectiveness make them viable alternatives to noble metal structures such as gold and silver [4,5].

At the nanoscale, copper exhibits size- and shape-dependent modifications in mechanical, electronic, and optical properties [6]. These variations arise from surface energy anisotropy, atomic coordination, and quantum

confinement effects. Understanding such behaviors requires simulation techniques capable of representing cohesive interactions and many-body effects intrinsic to metallic bonding. Classical interatomic potentials—including the Embedded Atom Method (EAM) and the Gupta potential—have proven effective in modeling metallic systems where bonding originates from delocalized electrons [7,8].

The Gupta potential, based on the second-moment approximation of the tight-binding model, includes both pairwise repulsive interactions and many-body attractive terms [9]. It has been widely employed to study nanostructures such as nanoparticles, nanowires, and nanosheets [10,11]. For copper, Gupta parameters are optimized to reproduce essential bulk properties, such as cohesive energy, lattice constants, and elastic moduli, while maintaining computational efficiency for large-scale molecular dynamics (MD) or Monte Carlo simulations [12].

2. METHODOLOGY

2.1 Model Construction

The computational model consists of a copper nanosheet oriented along the (110) plane and containing 221 atoms. The outermost atomic layers are fixed to serve as grips during stretching simulations, while inner atoms are allowed to relax. Atomic positions are initialized using the FCC lattice with appropriate lattice parameters, ensuring structural symmetry before optimization.

2.2 Simulation Using Gupta Potential

The system is modeled using the Gupta potential as shown in equation 1, which effectively captures n-body metallic bonding. The potential extends interactions up to the fifth-neighbor shell and accurately reproduces a wide range of copper properties, including phonon dispersion and high-temperature thermodynamics. During simulations, the nanosheet is subjected to incremental tensile strain under both single- and double-sided stretching conditions.

$$V = \sum_{i=1}^{N} \left[\sum_{j=1}^{N} A\exp\left(-p\left[\frac{r_{ij}}{r_o} - 1 \right] \right) - \sqrt{\sum_{j=1}^{N} \xi^2 \exp\left(-2q\left[\frac{r_{ij}}{r_o} - 1 \right] \right)} \right]$$

Equation 1: Gupta Potential Expression

2.3 Energy Minimization and Quasi-Static Stretching

Energy minimization is performed by iteratively adjusting atomic coordinates to locate the lowest-energy configuration. Tensile strain is applied quasi-statically by incrementally increasing the distance between the fixed grip layers. After each strain increment, inner atoms are allowed to relax until the system reaches a new equilibrium state.

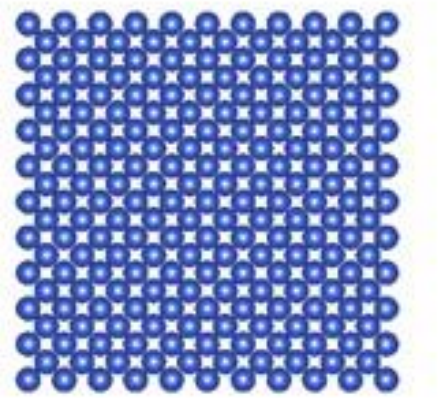

Figure 1: Initial unrelaxed copper nanosheet structure (221 atoms).

3. RESULTS AND DISCUSSION

During relaxation, in figure 2 we have shown that the nanosheet undergoes geometric optimization, revealing the early formation of vacancies, followed by grain boundaries as strain increases. At higher elongations, the merging of vacancies forms larger holes that ultimately lead to sheet rupture. This structural evolution is consistent with previously reported studies on gold nanosheets [13,14].

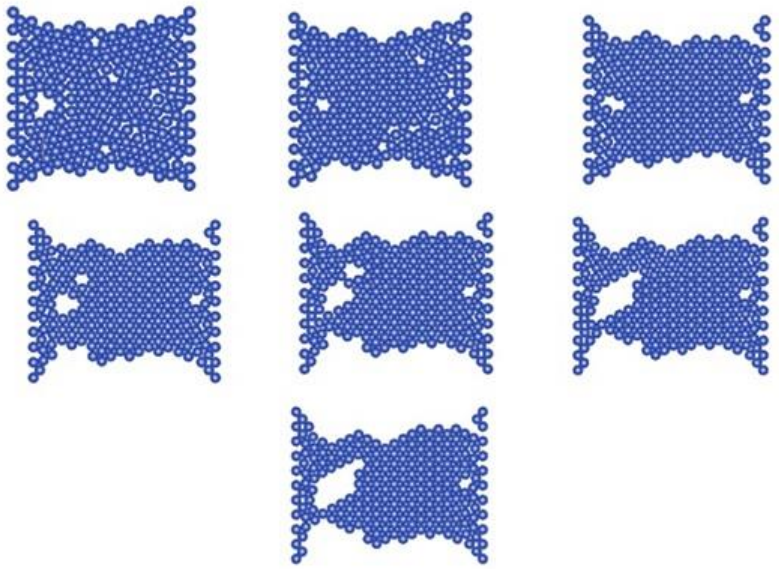

Figure 2: Vacancy formation and structural evolution during quasi-static stretching.

The onset of plastic deformation is characterized by rapid accumulation of defects, whereas regions not subjected to major deformation retain their crystalline order. These observations highlight the role of atomic coordination and cohesive forces in determining nanoscale mechanical behavior.

3.1 Energetics Analysis

In figure 3, the total energy increases monotonically with elongation until reaching a peak, signaling the elastic region which on further elongation will lead us to plastic deformation regions. The unphysical region beyond the plastic point represents states that cannot be sustained under equilibrium conditions.

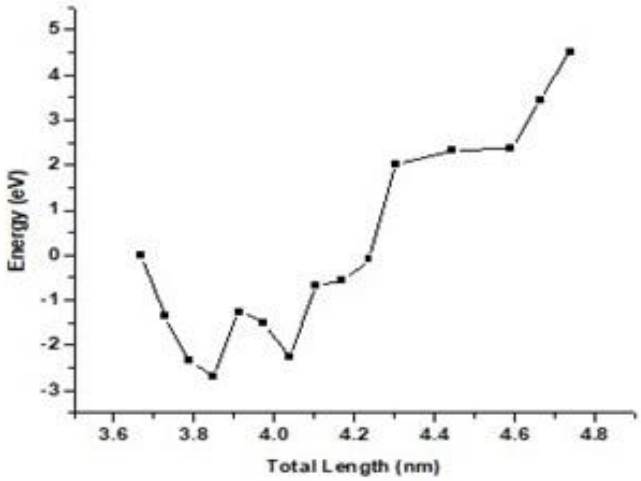

Figure 3: Total energy (U) vs total length (L) for the copper nanosheet.

4. CONCLUSION

This study demonstrates the effectiveness of the Gupta potential in modeling the structural response of copper nanosheets under tensile loading. The computational framework successfully captures vacancy formation, grain boundary evolution, and rupture behavior. These insights contribute to the broader understanding of mechanical stability in nanoscale metallic systems and provide a foundation for further exploration of vibrational, electronic, and optical properties of copper nanosheets.

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