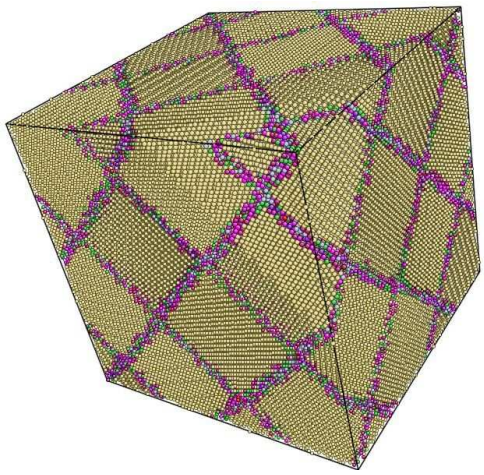
Molecular Dynamics Simulation of Sliding Friction

Numerical prediction of coefficient of friction and mixing at rapidly moving nanostructured materials interfaces

The Challenge

Understanding the mechanism underlining the nanoscale dynamic friction requires investigation of contact nanoidentation, experimental and analytical techniques. Materials in reality are not perfect, containing defects within the microstructure. The surfaces are inevitably rough and the real area of contact is actually a small fraction of the apparent area of contact. Thus, interfaces effectively adhere and the sliding is divided into the adhesion component and the so-called "ploughing" component, which is generated from the plastic deformation of the interfacial asperities.

Frictional sliding is a very complex process involving large plastic strains, which give rise to complex dislocation generation within the materials microstructure. Our purpose is to investigate the aspects of this complex process with the aid of molecular dynamic simulations. . A novel sliding friction simulation set-up is needed for nano-structured materials. Investigating the change of the yield point of the material under sliding friction and the accurate evaluation of the stresses involved has proved difficult and time consuming. This is primarily because the experiments are difficult to conduct and expensive facilities are required. Thus, exploring the fundamental rules governing the variation of materials strength is a very complex process.



Nanostructures copper: Visualisation of grains

The Approach

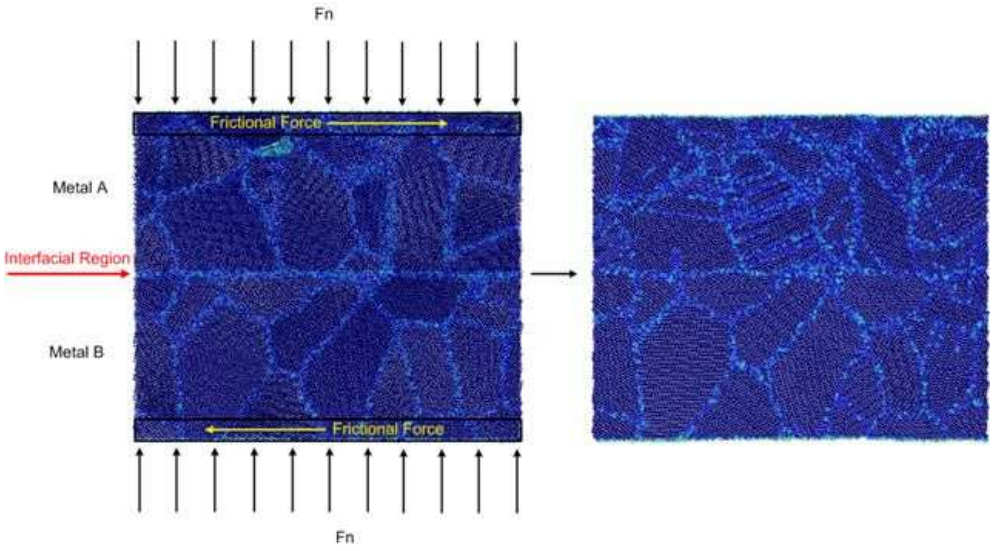
The Molecular Dynamics (MD) method is a deterministic simulation method that is based on the classical molecular model. Atoms are modelled as point masses whose interactions can be approximated by analytical potential functions. The atomic motion is governed by Newton's equation of motion given by

$$d^2\left(m_i r_i\right)/dt^2 = -\nabla_{r_i} V \ ,$$

where r_i is the position and m_i the mass of atom i. The system's potential energy, V, is the sum of the potential energies of all atoms of the system: $V = \sum_i V_i$.

The force on each atom i is thus $J_i = -\nu_{r_i} V$. The atomic trajectories can be calculated by using a numerical time integration method. Whether the simulation results are realistic depends mainly on the accuracy of the potential energy function. The MD simulations on high speed sliding have been performed with a normal pressure of 5.1GPa and sliding speeds sliding speeds of $v = 25, 50, 100, 150, 200, 300, \ldots, 1000$ m/s .

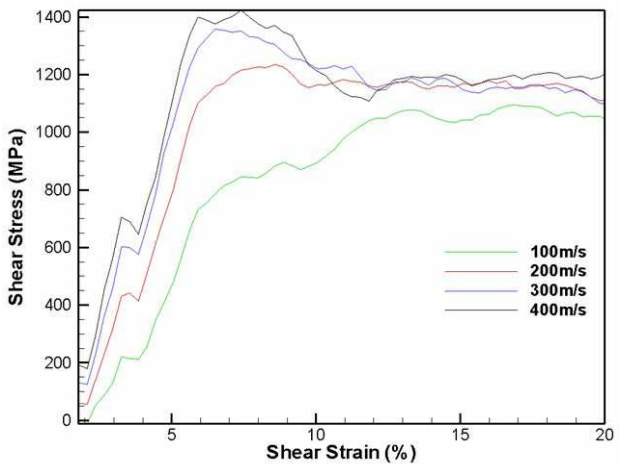
The set-up for the MD simulations of sliding is illustrated overleaf. The upper slab is made of copper and the lower slab of silver atoms. Both slabs are perfect FCC lattices with smooth surfaces in contact on the (001) crystallographic planes and sliding was initiated in the [001] crystallographic direction. The simulation domain tested has size of (*x*, *y*, *z*) = (410, 320, 330) Å, containing approximately 2.9M atoms.



Schematic representation of simulation set-up: Average grain size of 15nm

The Results and Benefits

The outcome of this study is leading to development of understanding of yielding, deformation, failure and coefficient of friction measurements under conditions in which physical experiments are very expensive and in some cases impossible to conduct. The molecular dynamics techniques accurately verify the deformation mechanism at grain sizes of around 10-15 nm and prove that the flow stress varies with grain size and is consistent with the Hall-Petch relation.



MD methods enable us to investigate various other phenomena related to friction and wear such as atomic diffusion and material mixing in the proximity of the interfacial region. Typical applications are ballistic penetration modelling and high speed machining.

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