Modelling the erosion of metal surfaces by ion bombardment

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Surface topography development induced by multiple impacts on gold is investigated by way of a hybrid Molecular Dynamics - on-the-fly kinetic Monte Carlo technique, enabling realistic time scales to be simulated.

Traditionally Molecular Dynamics (MD) simulations of multiple particle impacts have been carried out by modelling the ballistic phase with MD followed by a relaxation stage, and so on. Due to the time scale limitations of MD this does not allow for diffusion between impacts and can lead to an unrealistic build up of defects in the system.

Here a multi time scale technique is applied to the same problem. MD is used to model the ballistic phase while on-the-fly kinetic Monte Carlo is used to model diffusion between events.

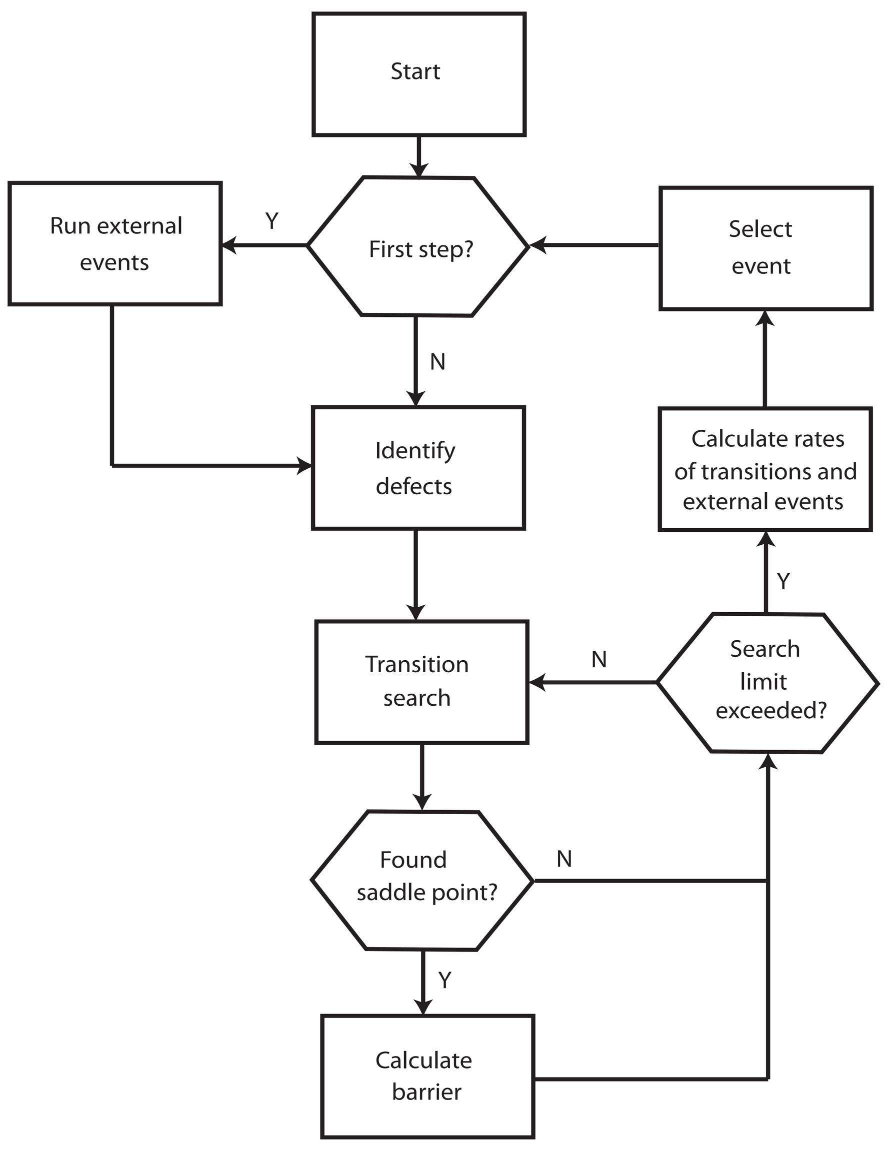
Methodology

Ar and Au 500 eV bombardment of an Au target with {0 1 0} surface orientation was considered.

The target contained 8,000 atoms with surface dimensions 4.1 x 4.1 nm^2.

The simulations were performed at 350 K using a Berendsen thermostat. Au and Ar self interactions were modelled using the Ackland and Lennard-Jones potentials respectively. Ar-Au was modelled with a repulsive ZBL potential.

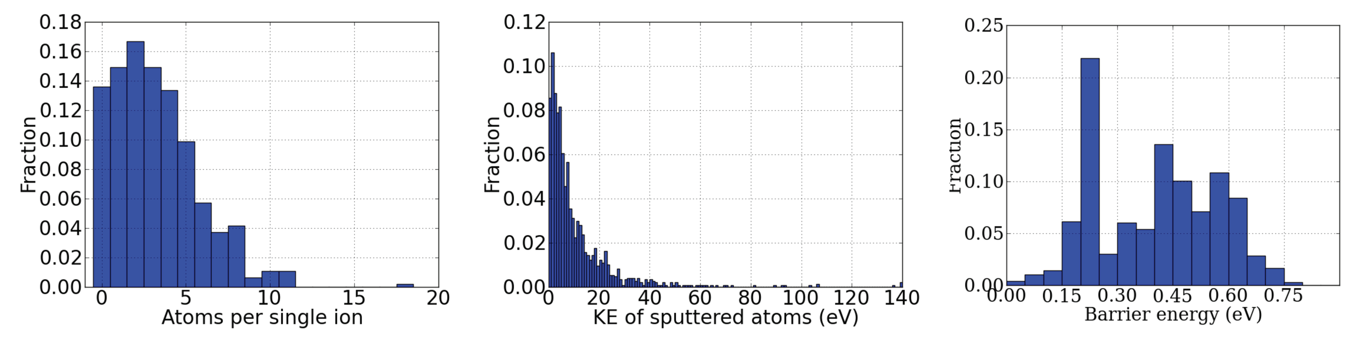
The RAT method was used to search for transitions and the NEB method to calculate the barriers. Bombardment events were performed in parallel with the transition searches.



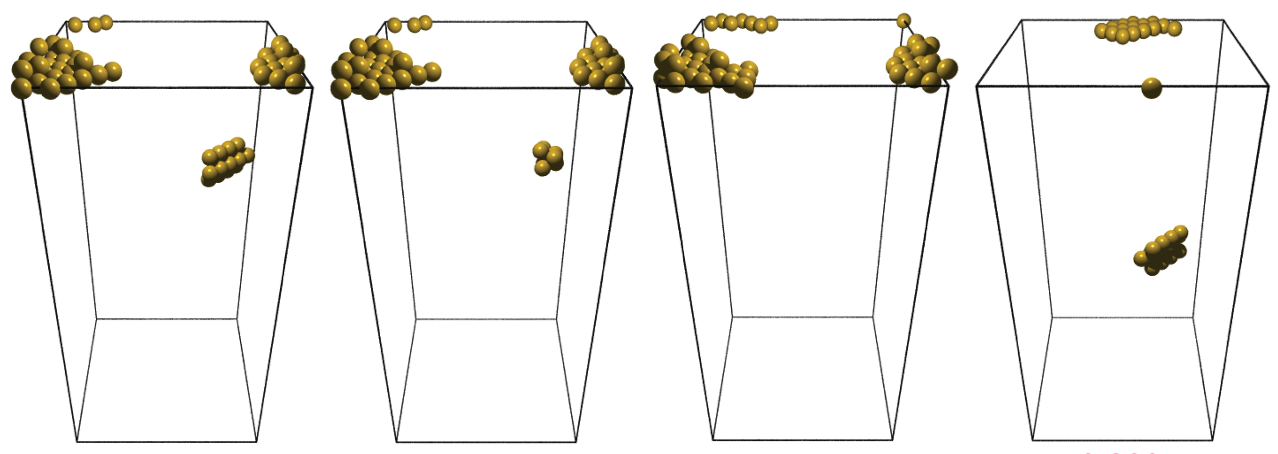
Au on Au bombardment

431 Au ions bombarded an 8,000 atom target with surface dimensions 4.1 x 4.1 nm. A simulation time of 0.854 s was achieved.

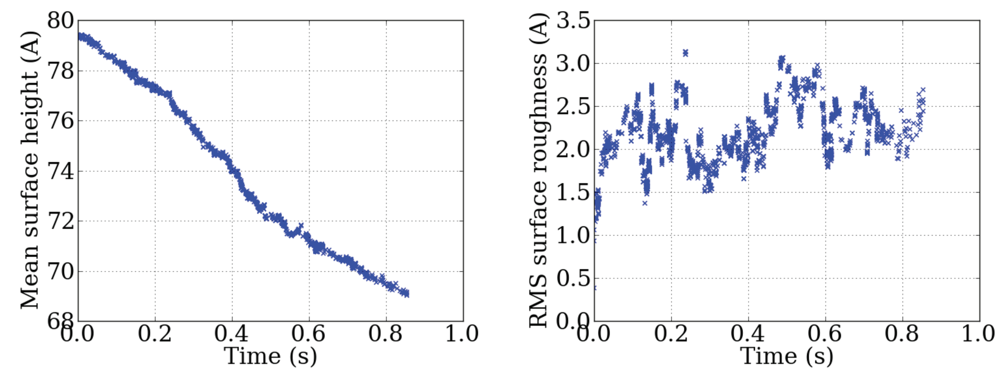
Below are graphs showing the distributions of the number of atoms sputtered per ion, the kinetic energies of sputtered atoms and the barriers for diffusion between events.



The images below show subsurface interstitials and adatoms above the height of the original surface. A large, immobile interstitial loop has formed in the first image. Following a single subsequent impact this loop has decayed to a much smaller loop that, after another further impact, has decayed completely. Later in the simulation another large interstitial loop forms. This process continues as the subsurface defects recover between impacts.



0.085 s 2.74 x10¹⁴ ions cm⁻² | 0.093 s 2.8 x10¹⁴ ions cm⁻² | 0.094 s 2.86 x10¹⁴ ions cm⁻² | 0.209 s 6.19 x10¹⁴ ions cm⁻²



The surface erosion rate is almost linear with time. Oscillations in the surface roughness are indicative of the healing process that occurs between bombardment events.

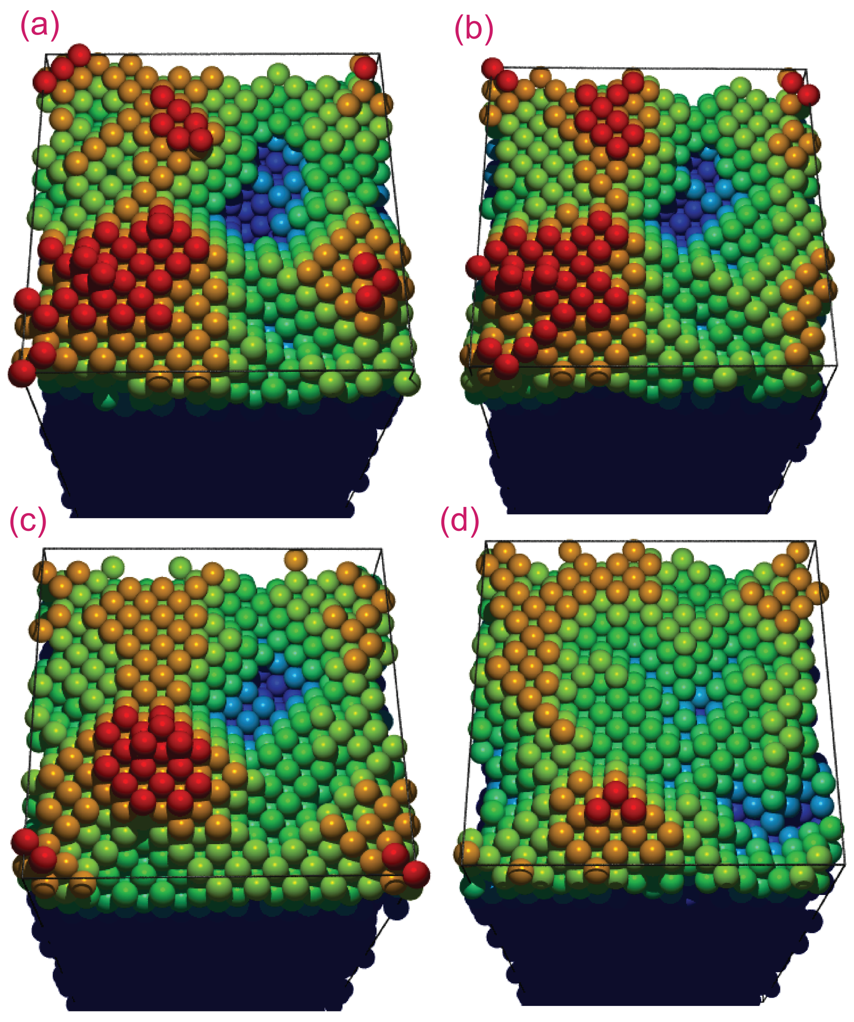
Ar on Au bombardment

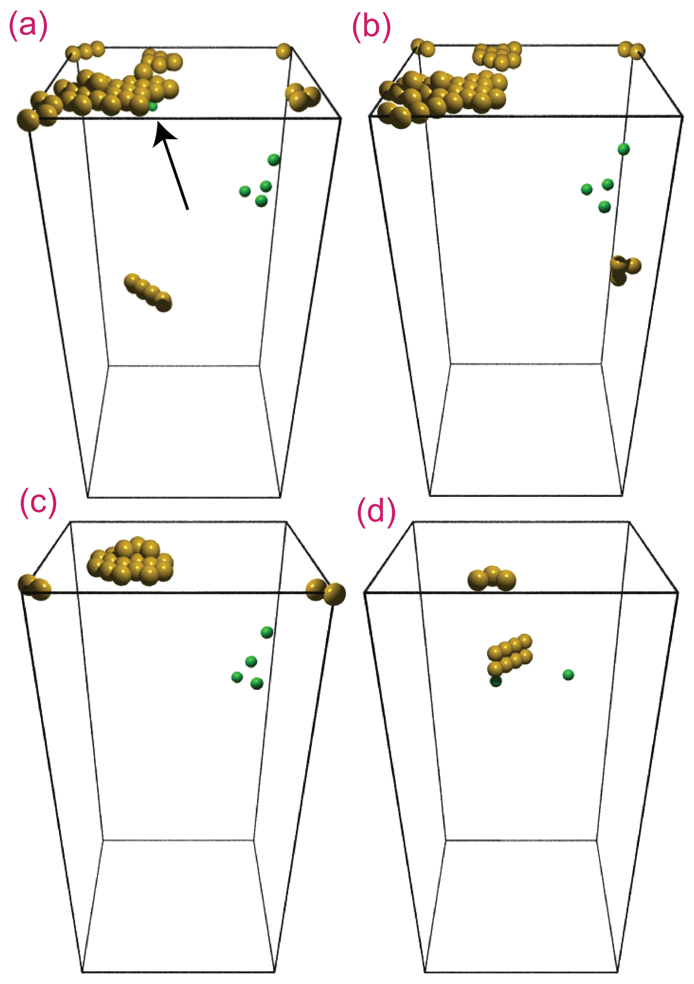
500 eV Ar bombardment of the Au {0 1 0} surface.

Images of the surface and corresponding sub-surface interstitials and implanted Ar atoms are shown.

(a) 0.085 s (2.38 $\times 10^{14}$ Ar cm^{-2})
(b) 0.087 s (2.56 $\times 10^{14}$ Ar cm^{-2})
(c) 0.090 s (2.74 $\times 10^{14}$ Ar cm^{-2})
(d) 0.137 s (3.69 $\times 10^{14}$ Ar cm^{-2})

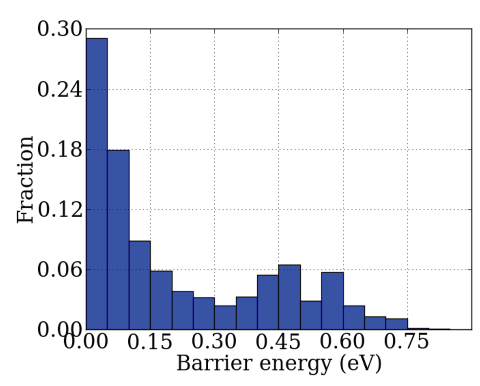
As the simulation progresses a rough topography forms as adatoms are thrown onto the surface and craters form. Healing occurs due to surface diffusion



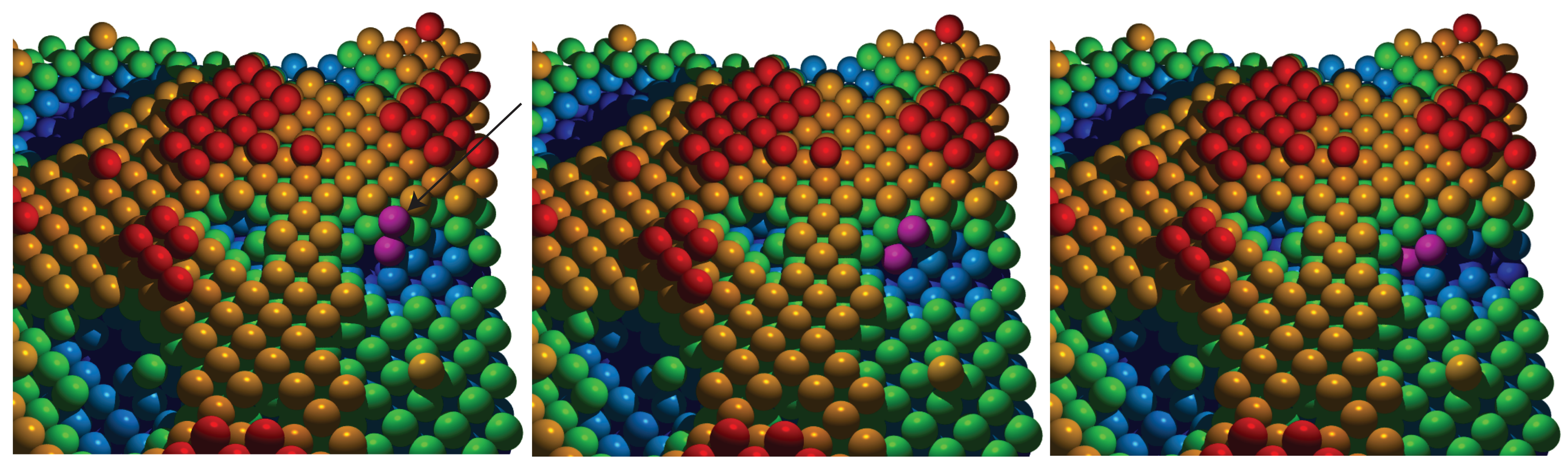


Subsurface interstitial loops form. Large loops remain immobile until they are annihilated by subsequent bombardments. Smaller loops of up to 5 atoms were observed to diffuse through the lattice.

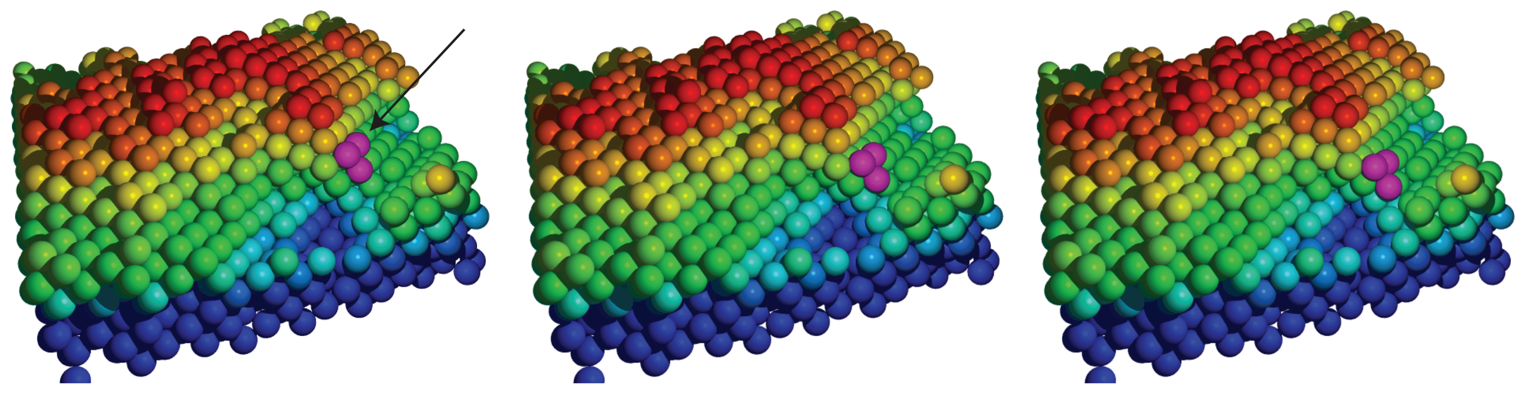
The large number of low energy barriers corresponds to subsurface diffusion of implanted Ar atoms.



Surface diffusion



A dimer of atoms (coloured purple) on the surface move together to fill a hole in the surface.



A trimer of atoms (coloured purple) move down a faceted crater edge, to a lower point.

Conclusions

Using our multi time scale technique we have successfully modelled surface erosion over realistic time scales. This model has highlighted the healing processes that occur between particle impacts, but occur on too long a time scale to be modelled by MD alone.

In all simulations we observe a rough topography form that stabilises as the healing process takes effect. The erosion rate of the surface was seen to be linear with time.

Subsurface interstitial loops are seen to form. Large loops of up to 17 atoms were immobile, however smaller loops of up to 5 atoms were observed to diffuse through the lattice.

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