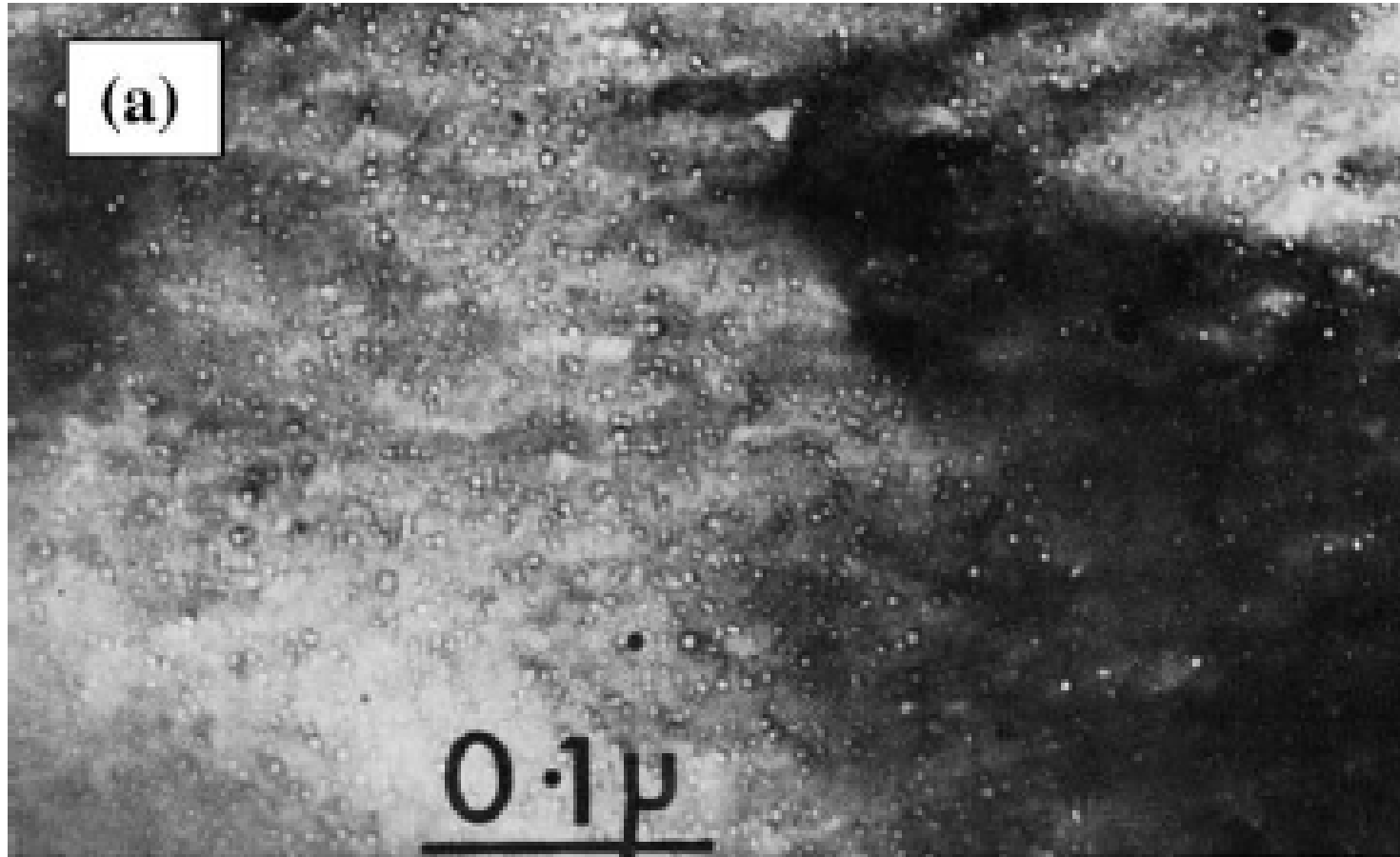
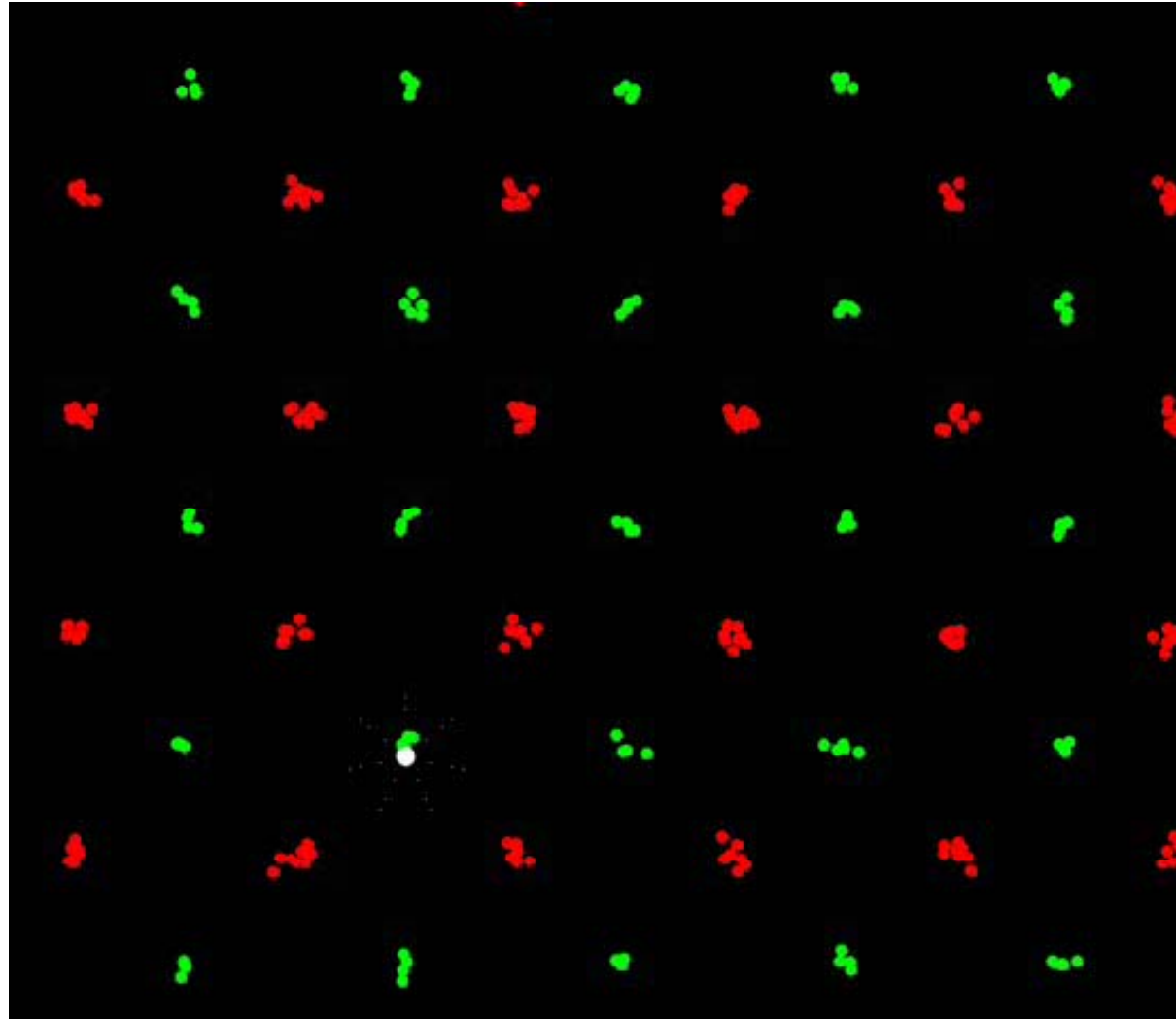


Molecular dynamics simulations of fission gasses in UO_2

David Parfitt and Robin Grimes



Olander *et al.*: J. Nuc. Mater. 354 94-109 (2006)



Aims of the study

- Develop a robust potential for the simulation of UO_2 and fission gasses. Must replicate:
 - High temperature behaviour and defect energies
 - Good core-core repulsion
- Apply this potential to look at behaviour of bubbles with respect to:
 - Bubble size
 - Fission gas pressure
 - Temperature of material
 - Recoil energy