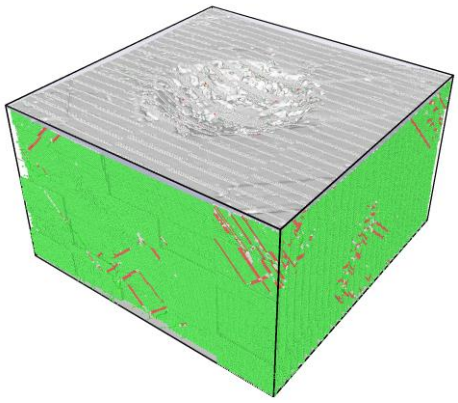
Atomistic Modelling of High Entropy Alloys

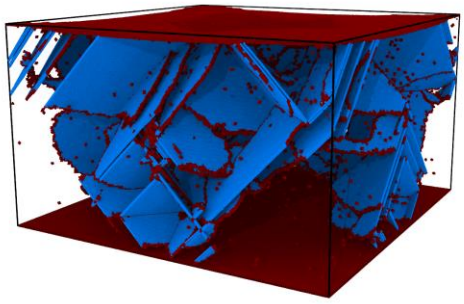
Akinjide Oluwajobi, Jan Ocenacek

New Technologies - Research Centre, University of West Bohemia, 30100 Pilsen, Czech Republic

High Entropy Alloys (HEAs) exhibit exceptional physical and mechanical properties for potential applications in many industrial sectors. To efficiently explore these multicomponent alloys, fundamental understanding of their deformation behaviour is essential.



Indentation of CoAlCuFeNi



Defect networks during indentation

As example, the Molecular Dynamics (MD) simulations of nanoindentation of CoAlCuFeNi was conducted, by using Embedded Atom Method (EAM) interatomic potential. These simulations reveal the nanoscale mechanisms of plasticity, critical to their excellent properties. The nanoidentation investigation shows dislocation evolution, cross-slip and twinning as the major mechanisms of plastic deformation.