Thermomechanical behaviour of nanocrystalline $(CoCrFeMnNi)_{1-x}Ni_x$ Complex Concentrated Alloys

Shankha Nag*
Karsten Albe
Otto-Berndt-Str. 3
64206 Darmstadt
*shankha.nag@tu-darmstadt.de

TECHNISCHE UNIVERSITÄT DARMSTADT

This project is funded by
DFG Project 388675407

material modellierung

Overview

Key Point of Enquiry: Role of changing Ni content on grain boundary state and deformation behaviour in $(CoCrFeMnNi)_{1-x}Ni_x$ polycrystals.

Reason for chosing $(CoCrFeMnNi)_{1-x}Ni_x$ series?

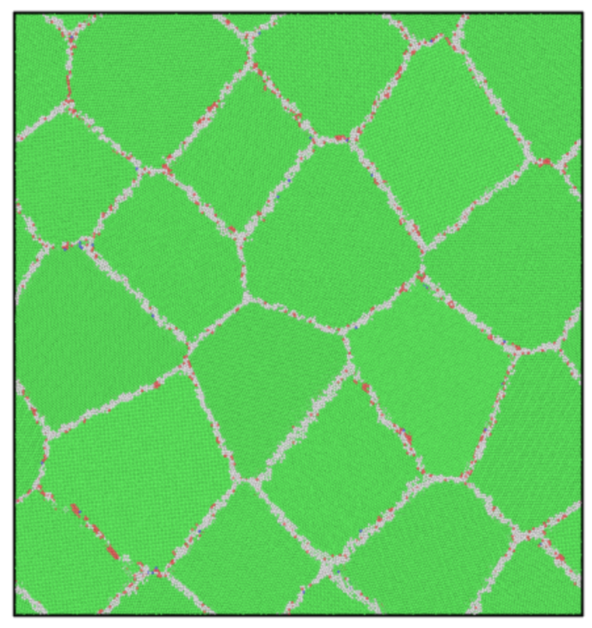
1. Experimentally, the alloys in the series are known to crystallize into fcc. So we can stick to a single crystal structure in our simulations.
2. It's known that *stacking fault energy* transitions from *negative in cantor alloy* to *positive in pure Ni*; leading to changing deformation mechanism with varying Ni content.
3. Role of *grain boundary state on deformation* is yet not fully explored in these systems.

Goals of the study

Using Molecular Dynamics and Molecular Statics with open-source molecular dynamics code LAMMPS

1. Study deformation mechanisms via uniaxial tensile testing.
2. Calculate grain boundary energy and stacking fault energy.
3. Calculate strain-rate sentivity and activation volume of stress relaxation in prior strained specimens.
4. Explore the microscopic mechanisms behind macroscopic deformation and then correlate them to intrinsic alloy properties like stacking fault energy.

Polycrystalline microstructure



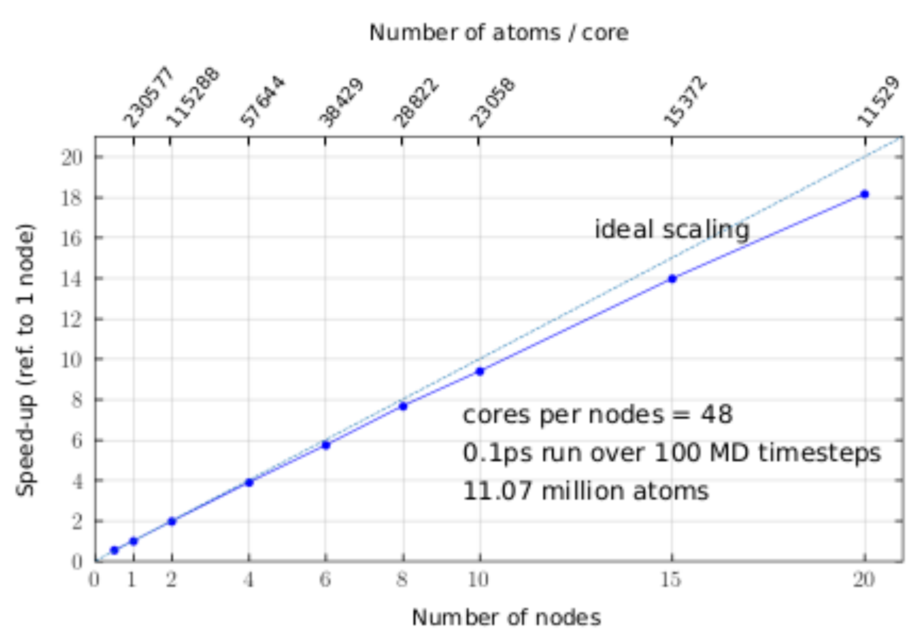
Periodic boundary conditions on all sides

54 grains
~ 11 million atoms

Different alloys are constructed by changing atom types
(microstructure kept fixed)

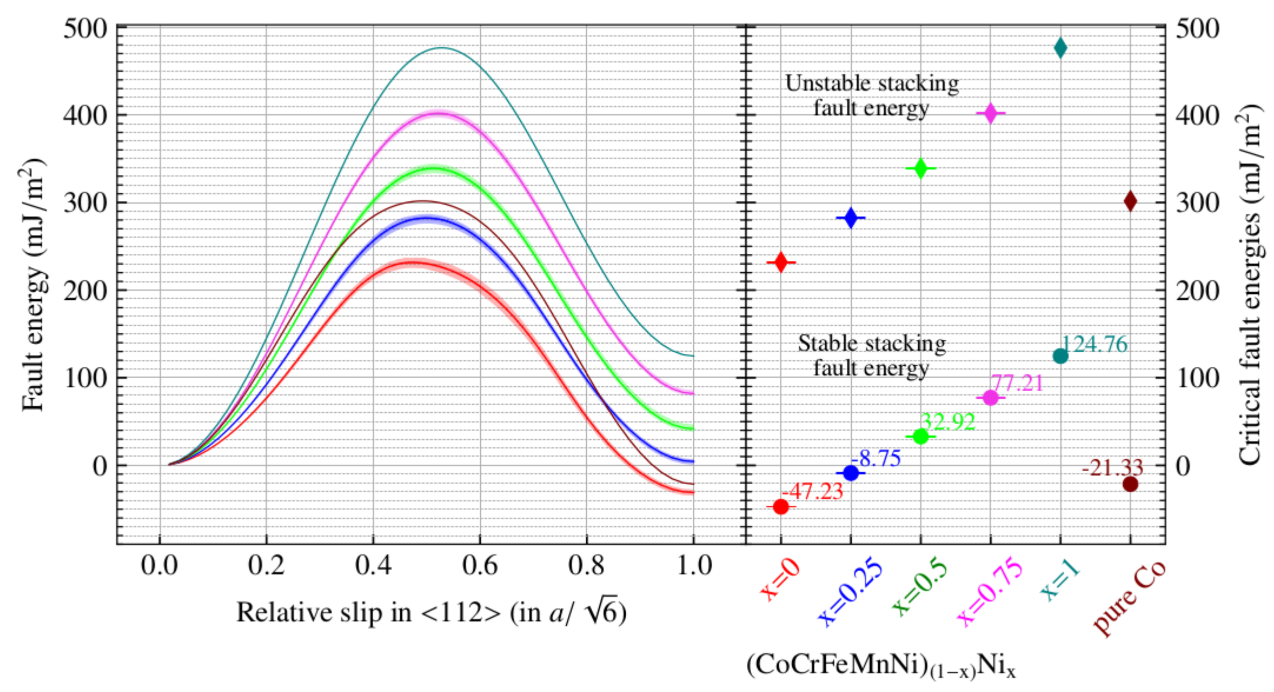
- fcc atoms
- hcp atoms
- disordered atoms

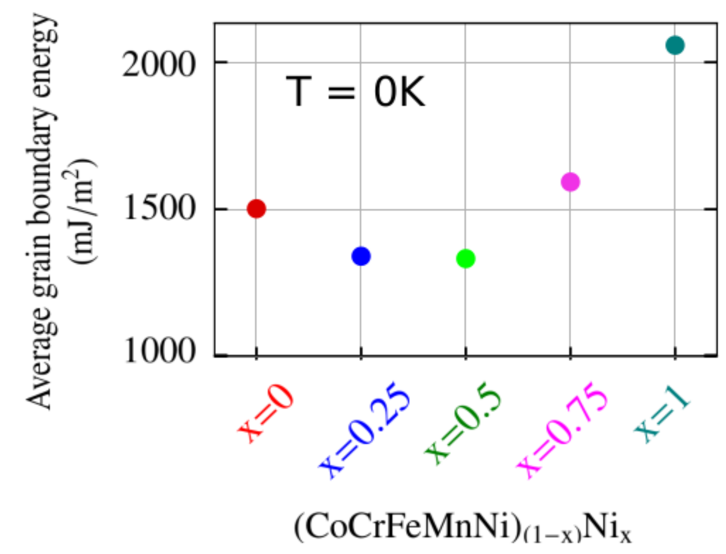
Code performance on JUWELS



Resource Allocation and Results

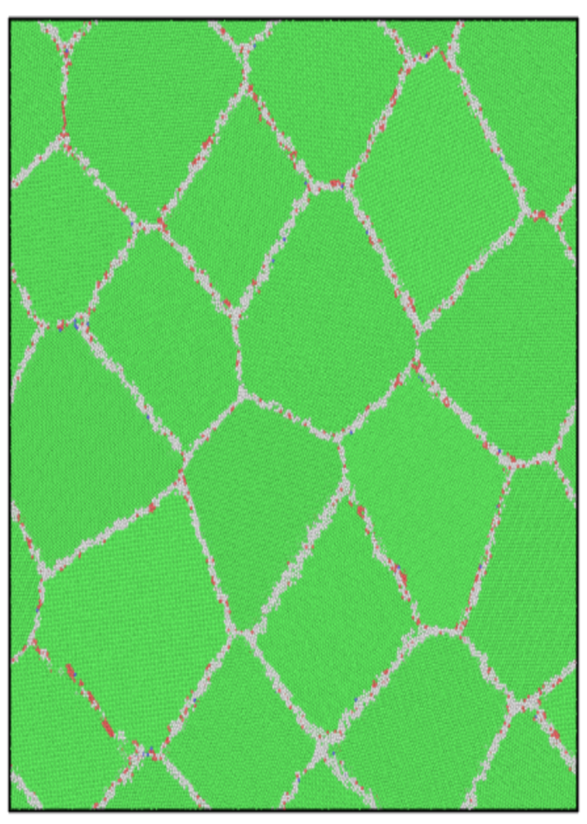
Grain boundary and stacking fault energies

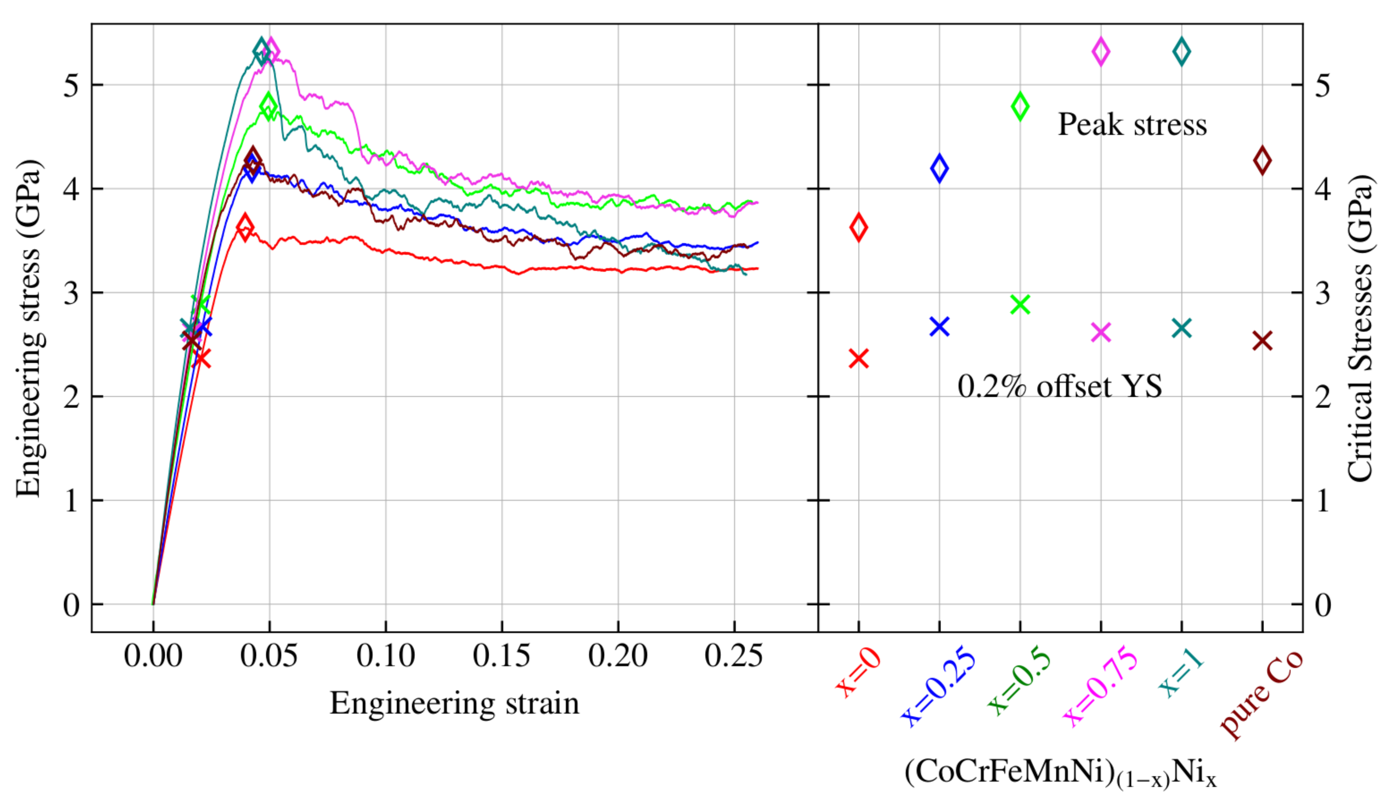


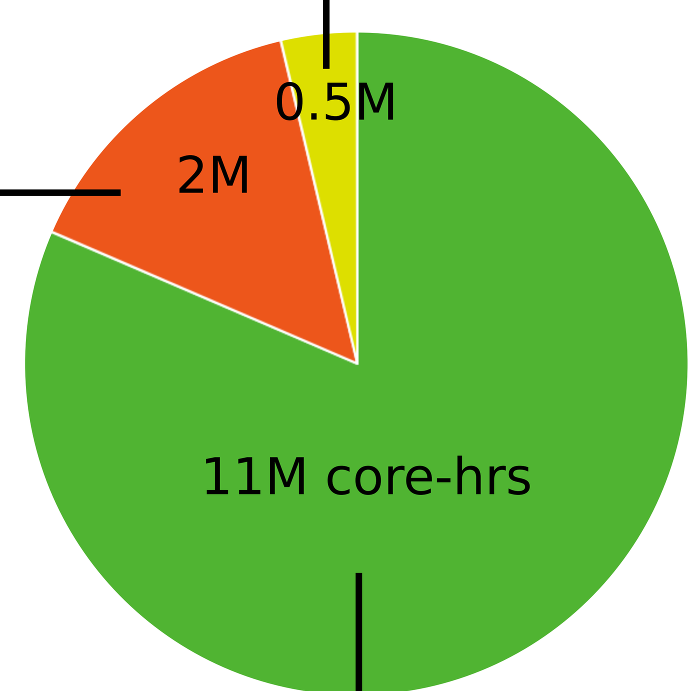


1. The trend of variation in unstable SFE is the same as the stable SFE (*Bell–Evans–Polanyi principle*).
2. SFE follows Vegard's law

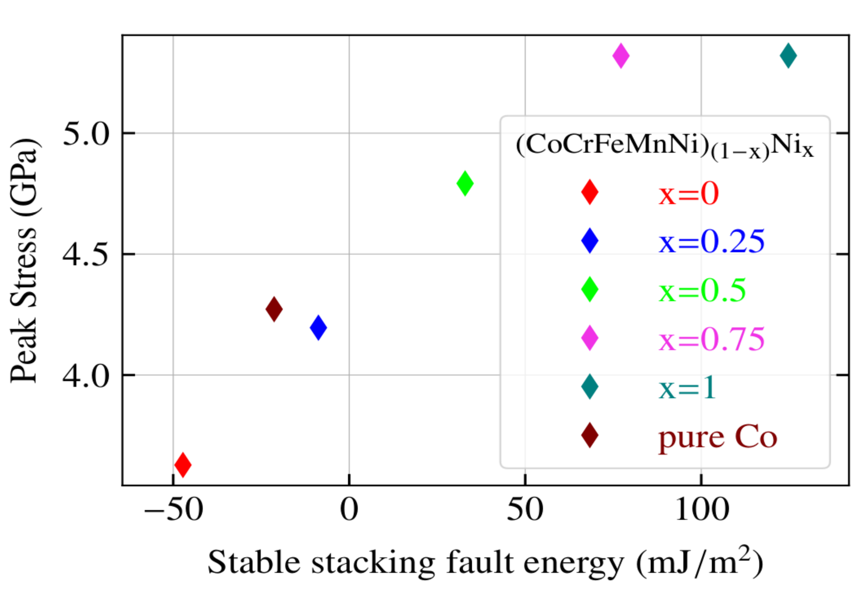
Uniaxial tensile tests



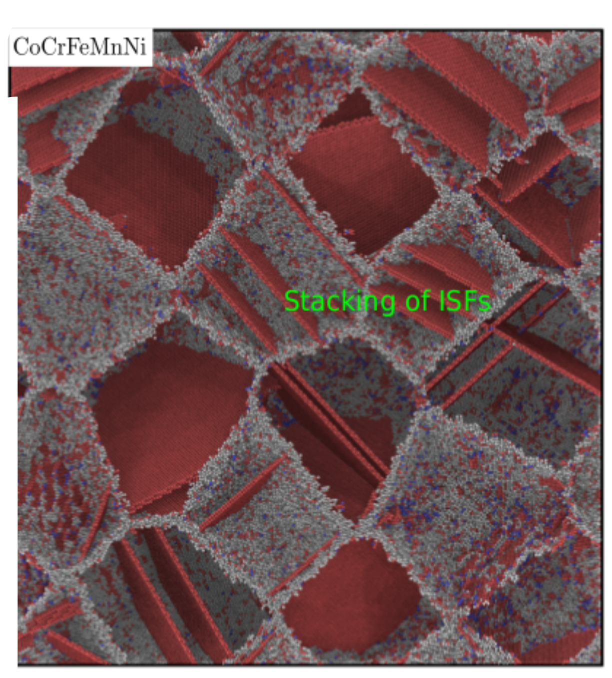




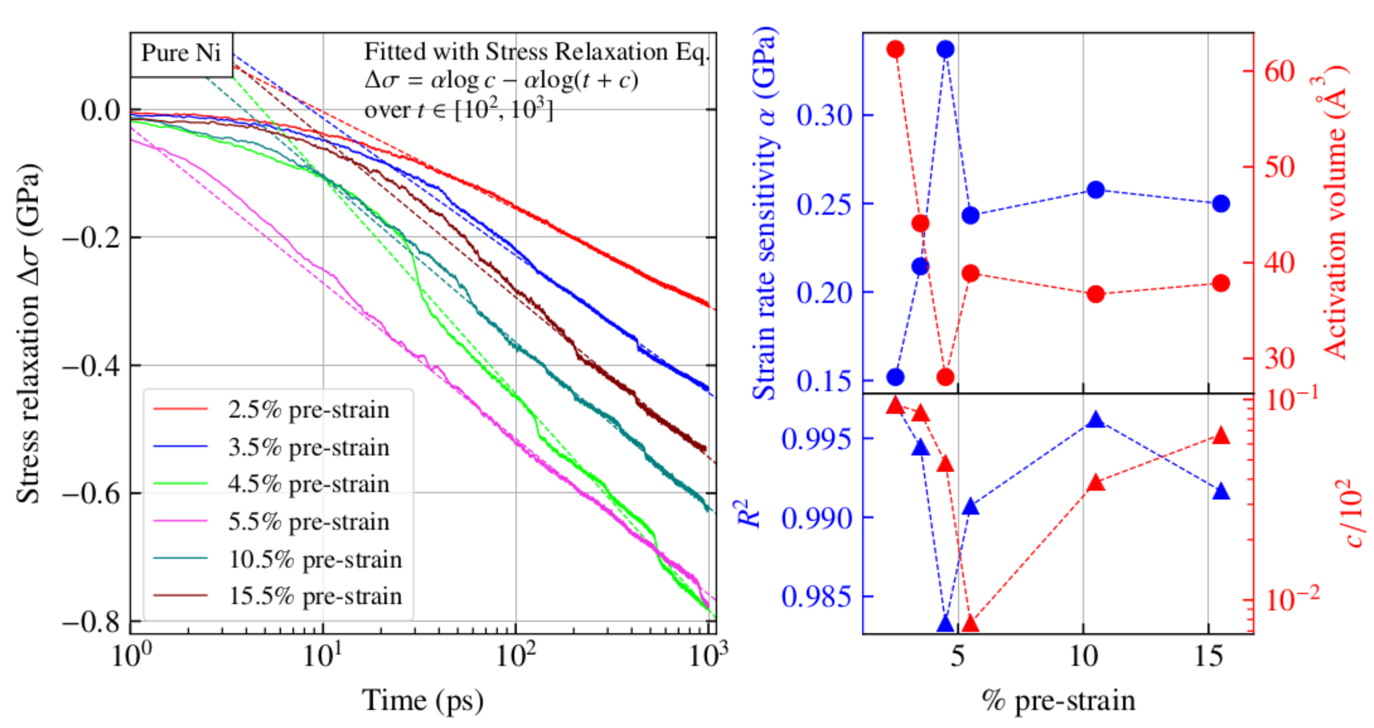
Strong correlation of stacking fault energy with peak strength

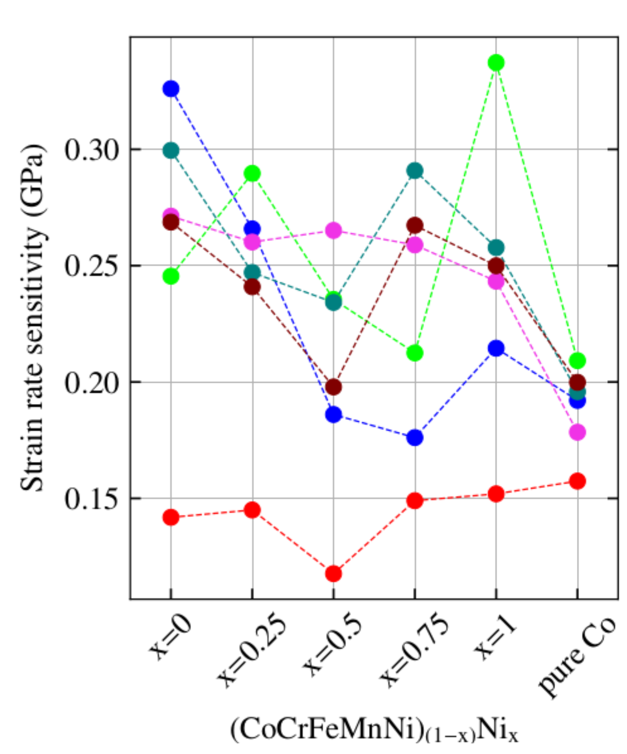


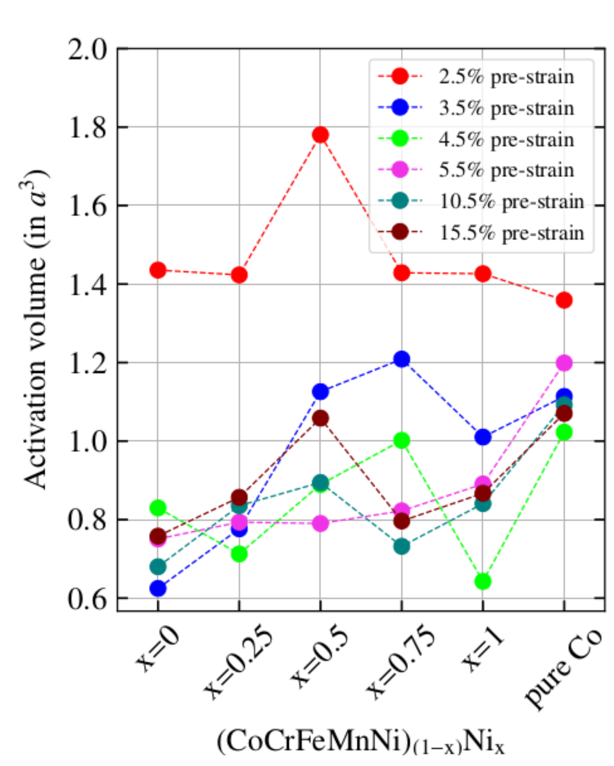
Emission of partial dislocations from grain boundaries at peak strength



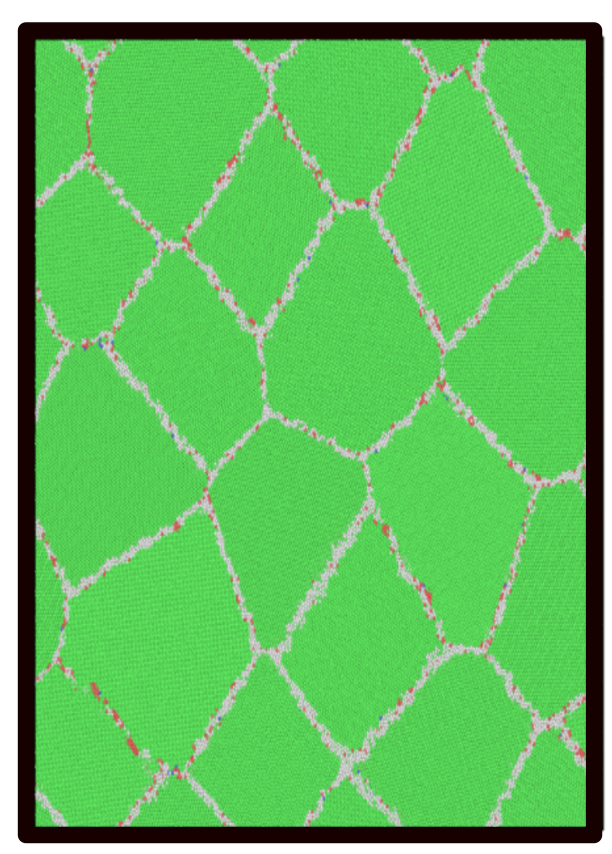
Peak stress controlled by partial emission from grain boundaries and accumulation of intrinsic stacking faults (ISFs) in the grains







Stress relaxation tests



Stress relaxation of lightly prestrained sample is mediated through grain boundary relaxation **(high activation volume)**

Stress relaxation of heavily prestrained sample is mediated through partial nucleation from the grain boundary **(low activation volume)**