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Semi-empirical interatomic potential for large-scale molecular dynamics simulation of metal-oxide systems

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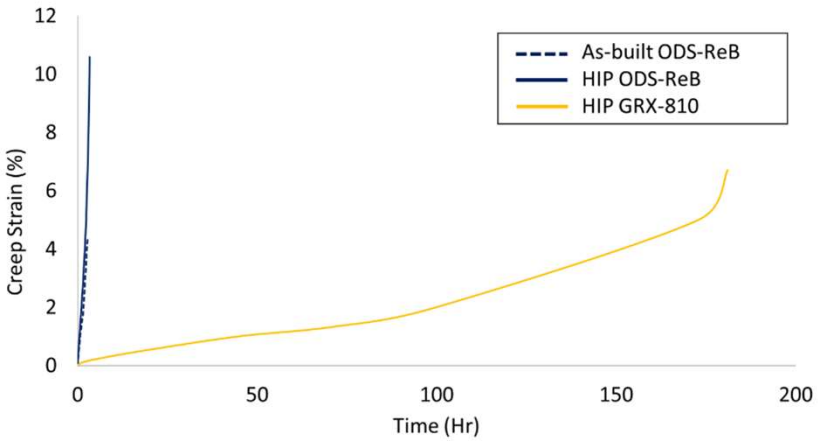
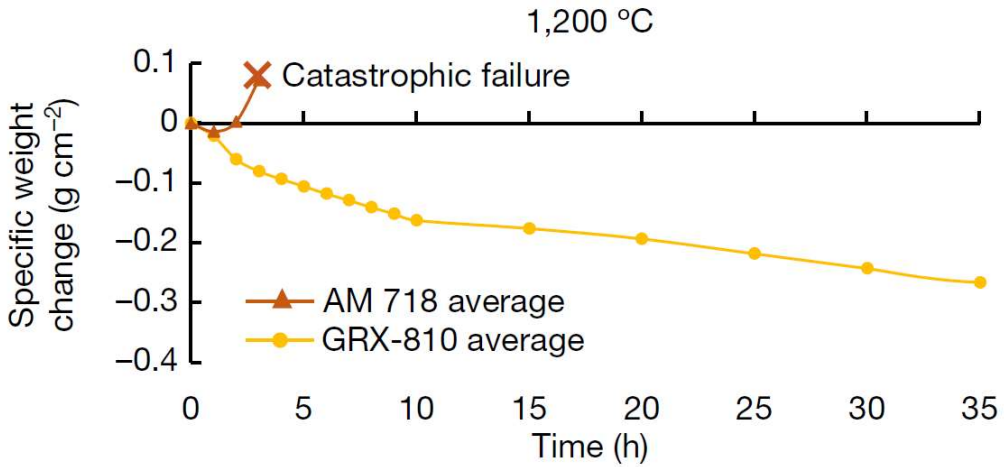
GRX-810 alloy[§]

Alloy	Ni	Co	Cr	Re	Al	Ti	Nb	W	C
GRX-810	bal.	33	29	1.5	0.3	0.25	0.75	3.0	0.05

Creep curves of ReB-ODS and HIP GRX-810 at 41 MPa / 1093°C.



Cyclic oxidation results for GRX-810 and superalloy 718



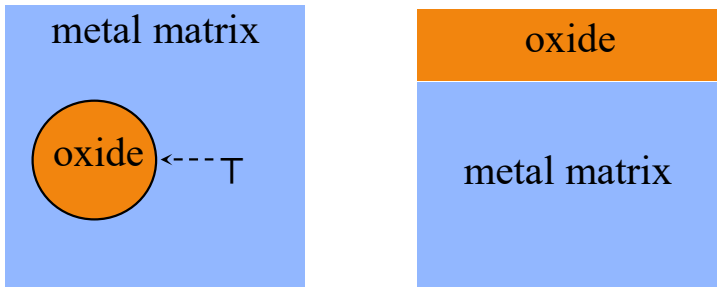
- GRX-810 is specially designed for AM.
- GRX-810 is providing orders of magnitude improvements in creep rupture life at 1093 °C compared to conventional superalloys 718 and 625.
- GRX-810 provides much better oxidation properties at 1200 °C compared to the superalloy 718.

- Molecular dynamics (MD) simulation must explain these results and provide a guidance for further alloy improvement.

[§]T.M. Smith *et al.*, Nature **617**, 513-518 (2023).

Requirements for interatomic potentials

Typical simulated systems



- Simulation cell should include an oxide-matrix interface and maybe dislocations.
- The Coulomb interaction must be considered.
- Atomic charges should depend on neighbor sphere chemistry (distance from the interface).

Large scale MD simulation: the description of interatomic interaction must be computationally cheap.

	Classical potentials	ML potentials
Agreement with *ab initio* atomic level information		
Target complex properties		
Easineness to develop		
Computational time		

Charge transfer ionic potential (CTIP)

Total energy: $E = E_{SEP} + E_{es}$

Electrostatic energy: $E_{es} = \sum_{i=1}^{N} \left[\chi_{t_i} q_i + \frac{1}{2} J_{t_i} q_i^2 \right] + E_C$

where χ_{t_i} and J_{t_i} are the electronegativity and atomic hardness.

Coulomb energy: $E_C = \sum_{\substack{i=1 \\ j=i+1}}^{N-1} q_i q_j \frac{1}{\left(r^3 + r_0^3 \right)^{1/3}}$

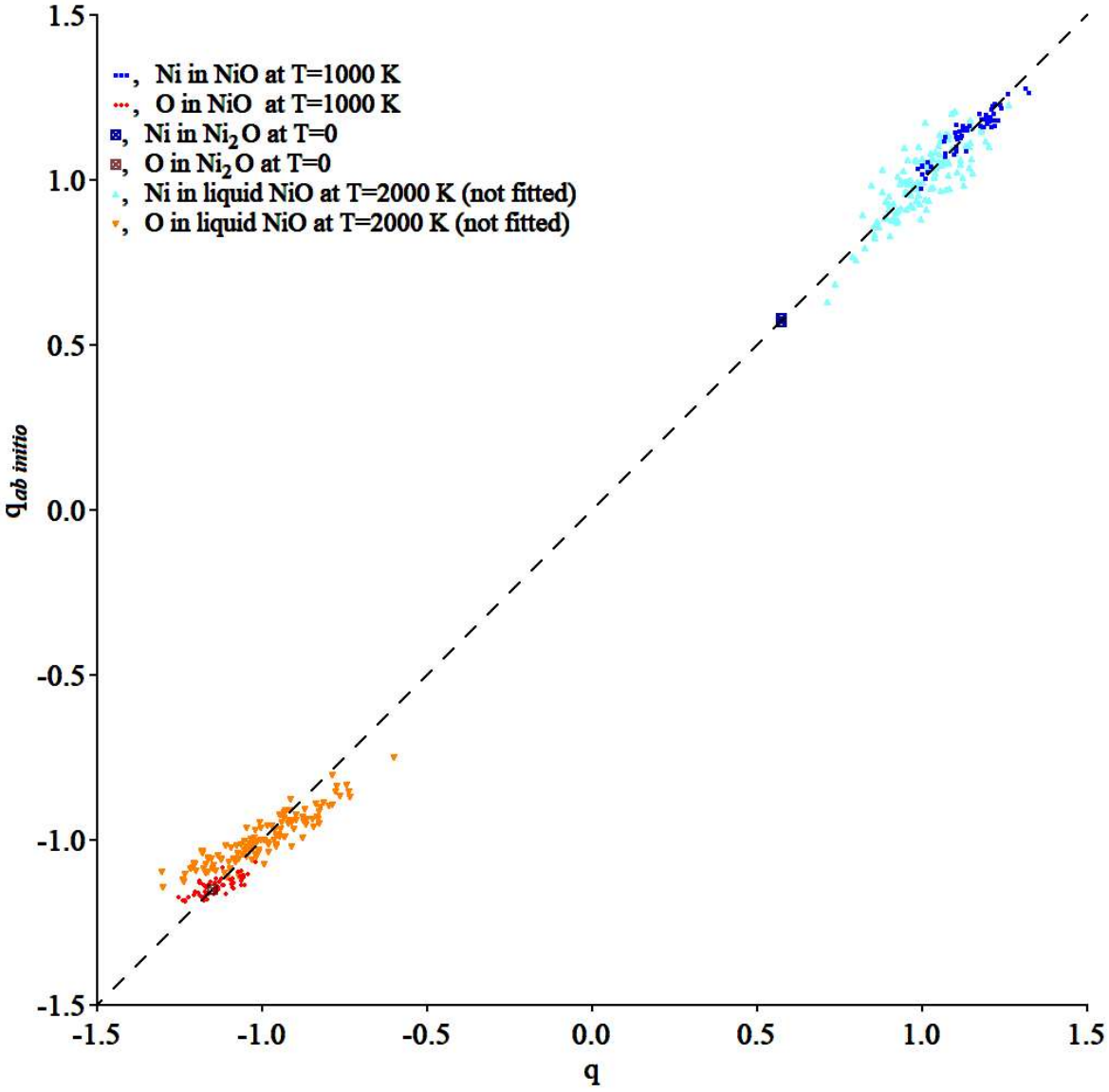
where r_0 is an empirical parameter to account for non-point charge distribution.

- Determination of the Coulomb energy requires the Ewald summation which can be avoided if the Coulomb potential is replaced by a shifted potential as proposed by D. Wolf[§].
- The only electrostatic parameters to fit are χ_{t_i}, J_{t_i} and r_0.
- The fitting of electrostatic parameters is decoupled from fitting of the semi-empirical potential.

- Ni-NiO system as the first step to simulate GRX-810.

[§]D. Wolf *et al.*, J. Chem. Phys. **110**, 8254-8282 (1999).

Fitting electrostatic parameters



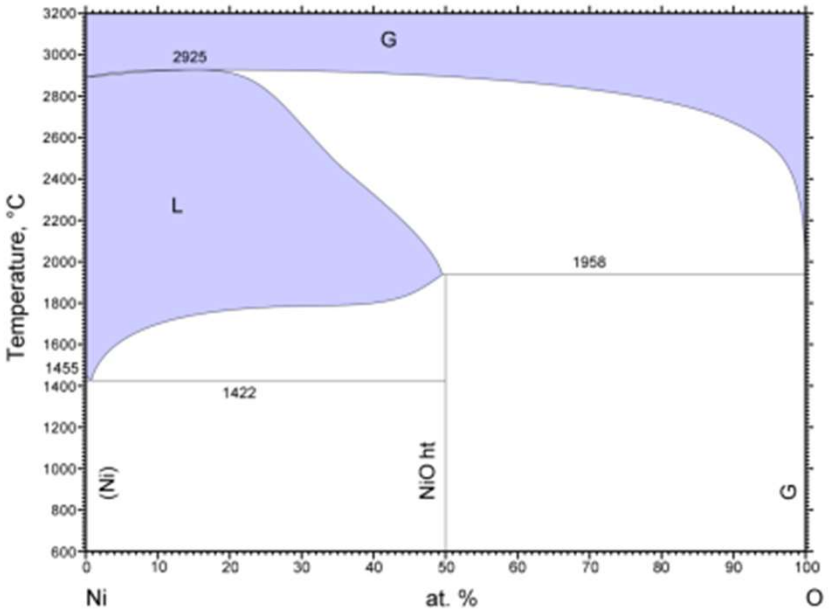
- The CTIP well reproduces *ab initio* data.

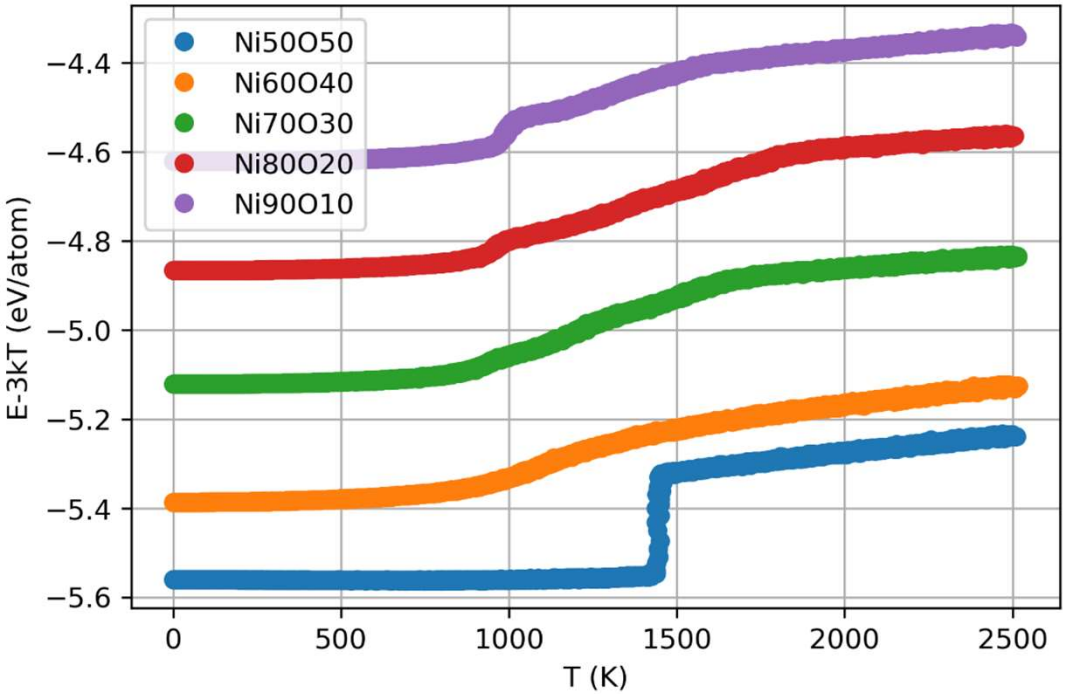
Solidification of NiO

The simulation cell contained ~50,000 atoms

Ni-O melt was equilibrated at 2500 K for 1 ns.

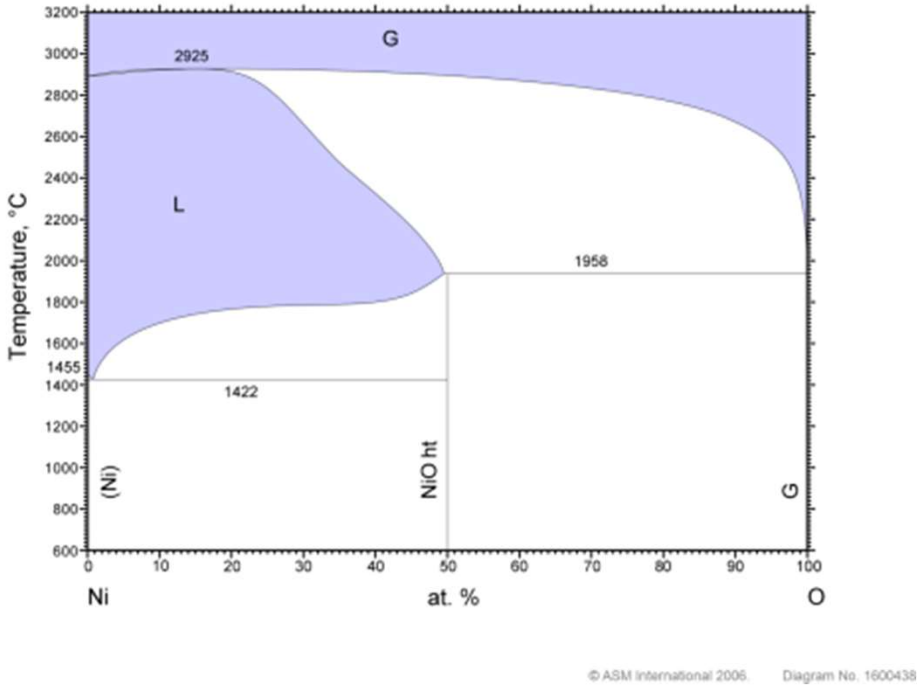
The system was cooled with $dT/dt=10^{12}$ K/s.

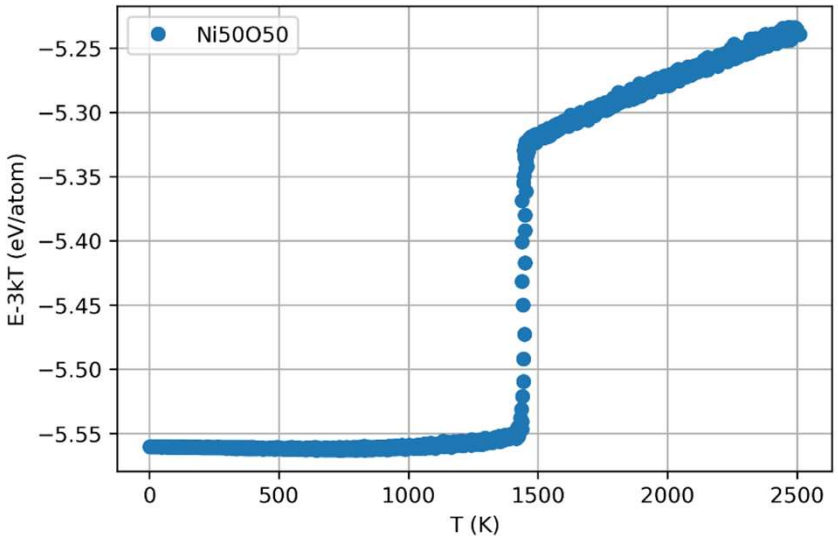


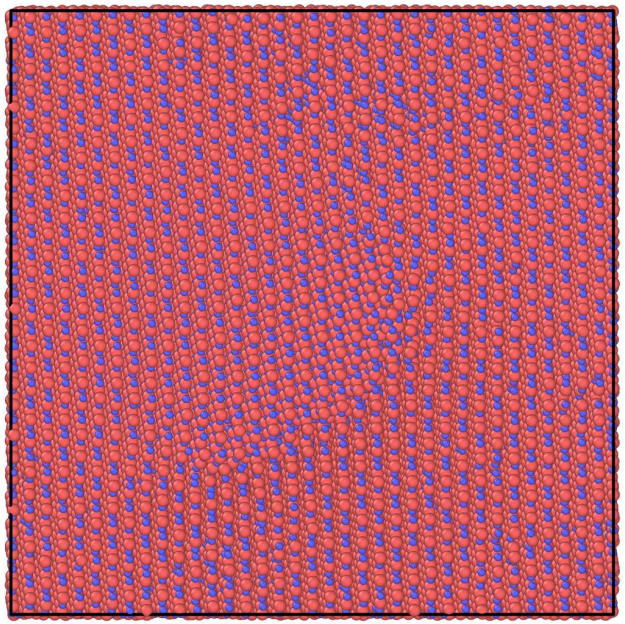


- Different solidification behavior was observed based on composition – crystallization, vitrification and phase separation – in agreement with the phase diagram.
- Processes during AM can be simulated.

Solidification of $Ni_{50}O_{50}$

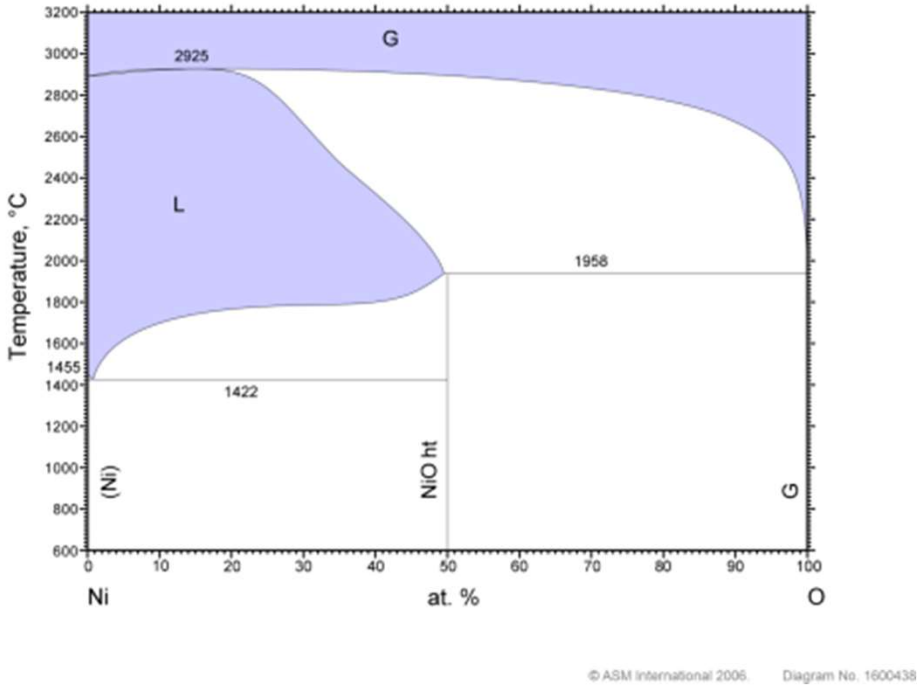


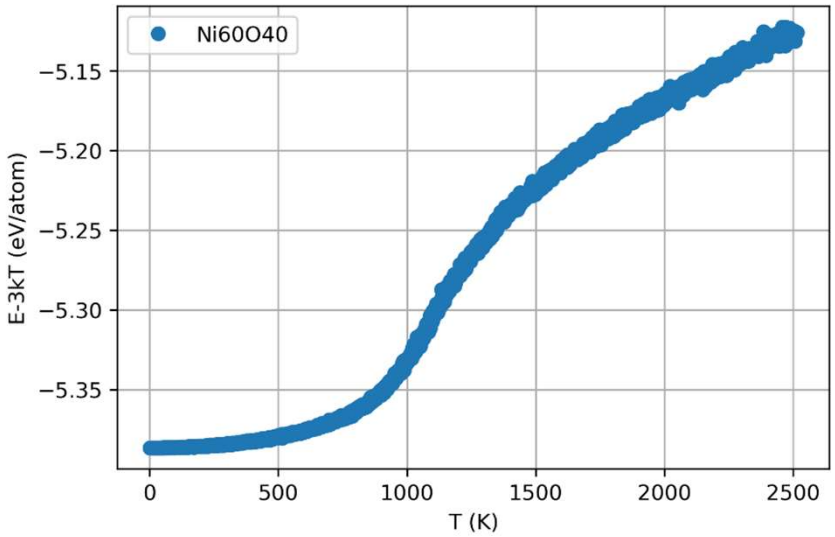


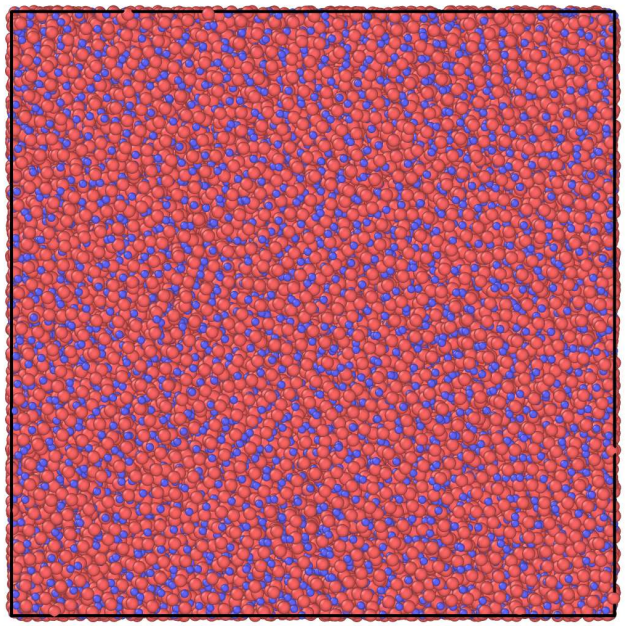


- Crystallization into the rock salt structure was observed.

Solidification of $Ni_{60}O_{40}$

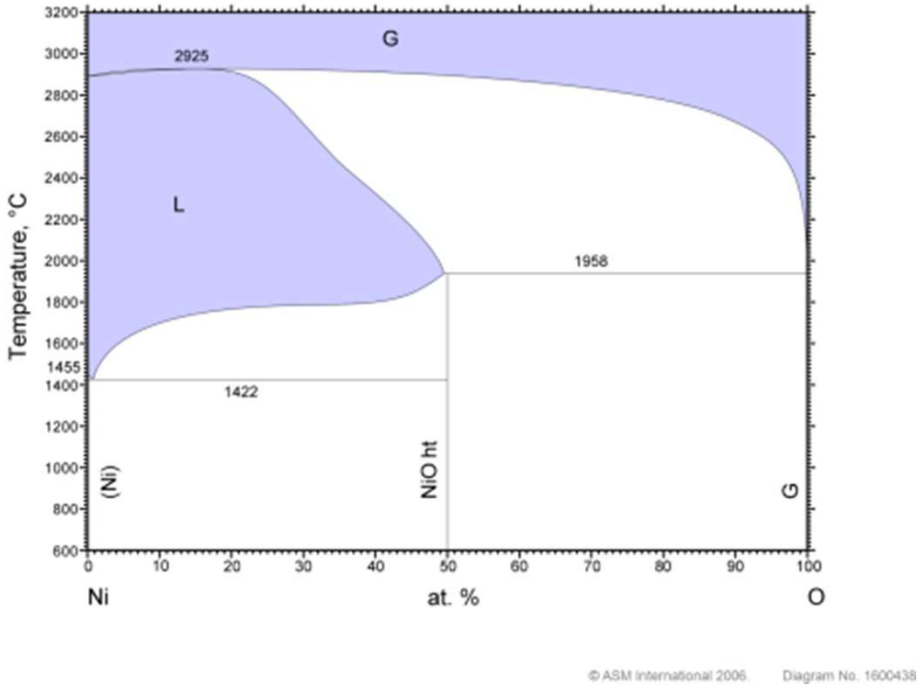


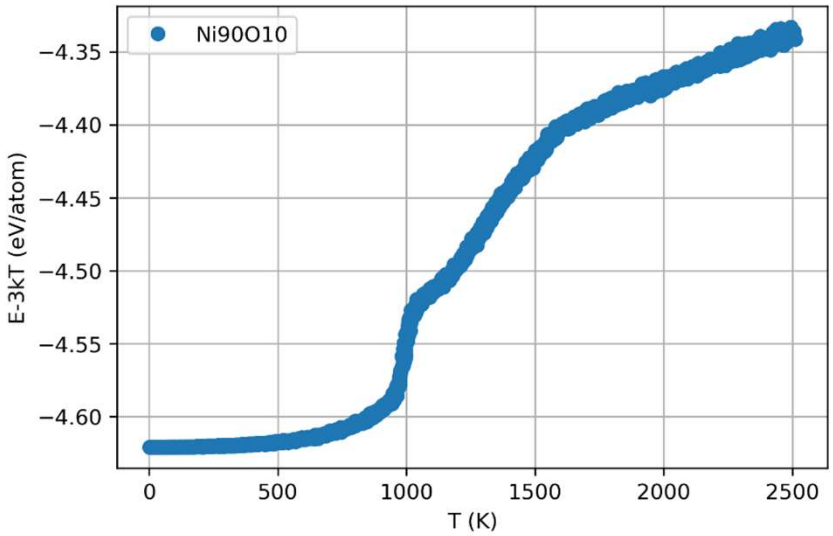


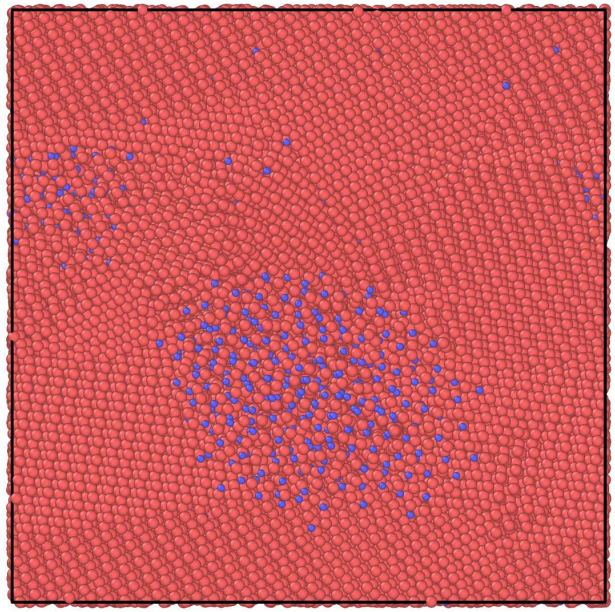


- Crystallization into an amorphous structure was observed.

Solidification of $Ni_{90}O_{10}$



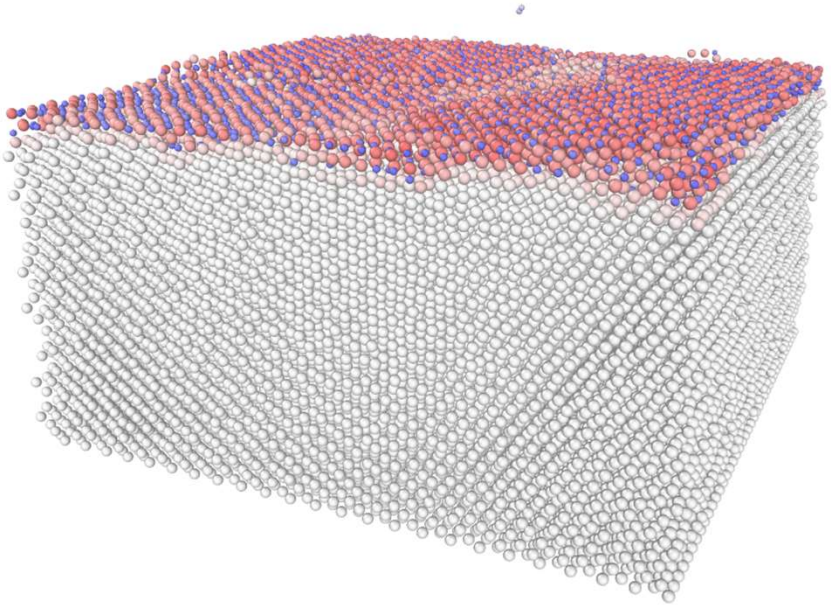


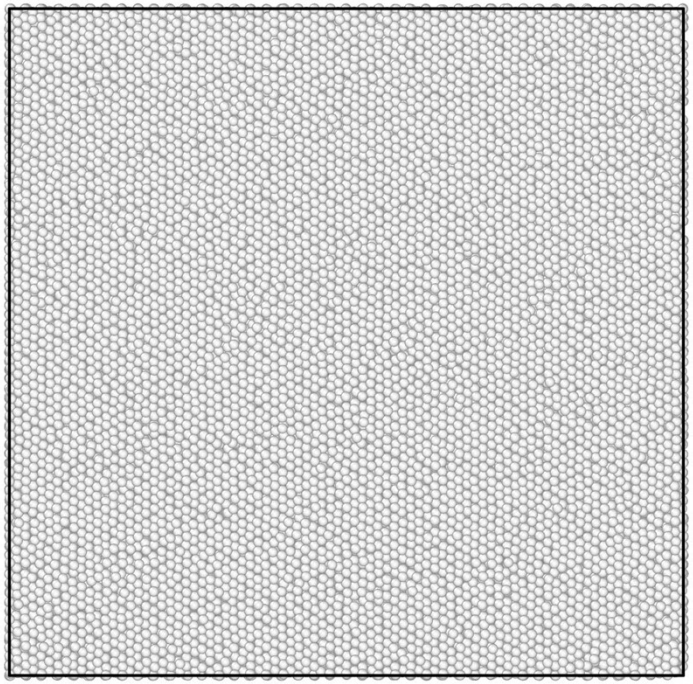


- Crystallization into a two-phase system was observed.
- No oxygen solubility in Ni was observed.

Ni oxidation

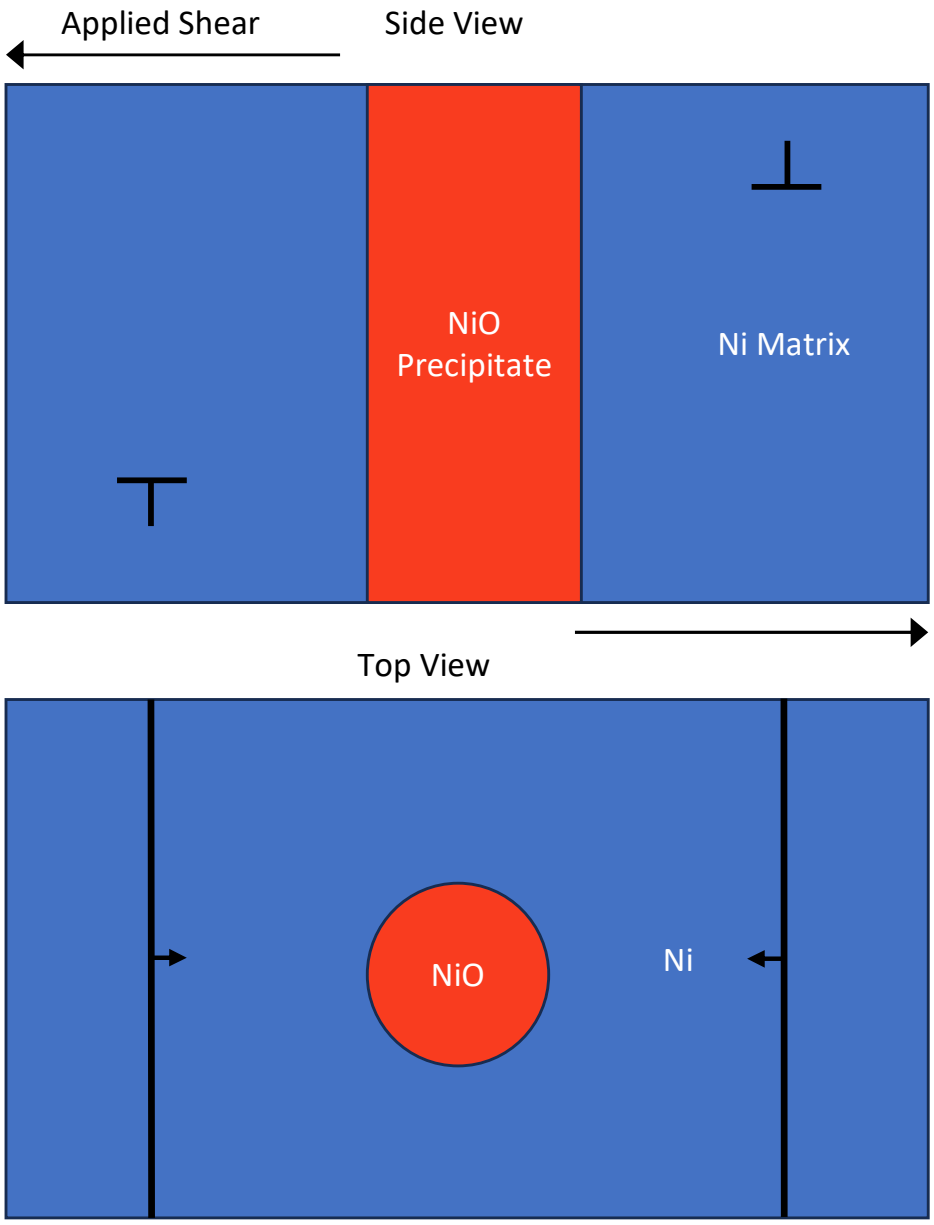
T=800 K
55,000 atoms
30 ns.



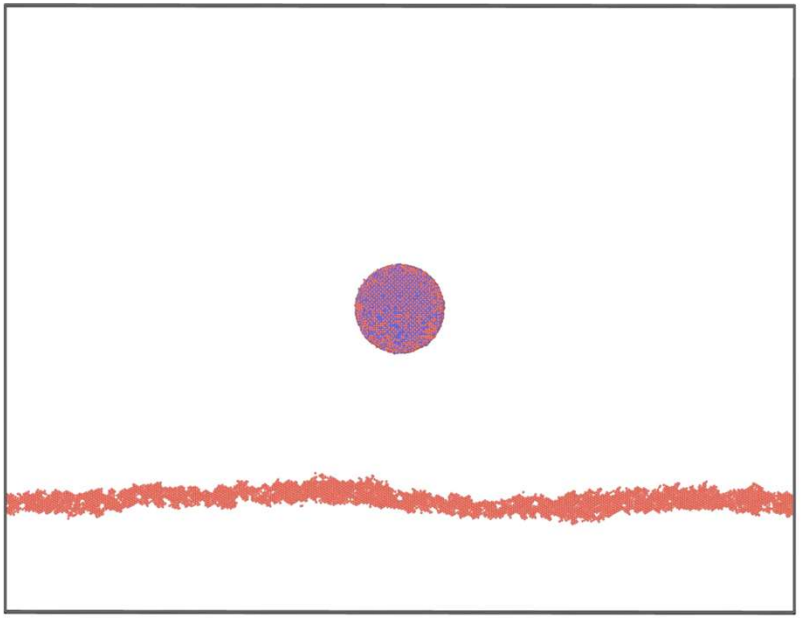


- Formation of a NiO oxide layer with the rock salt structure was observed.

Interaction between NiO particle and dislocation



T=1000 K
σ=100 MPa
13,000,000 atoms



- NiO particle is an obstacle for the dislocation migration.

Summary

- A CTIP for the Ni-NiO is developed.
- The developed CTIP allows to simulate the processes happening during AM.
- The developed CTIP allows to simulate the Ni oxidation.
- The developed CTIP allows to simulate the creep resistance of the oxide strengthened Ni.