



Atomistic Simulations of Early-Stage Oxidation Mechanisms in Oxide Dispersion Strengthened Alloys

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Overview

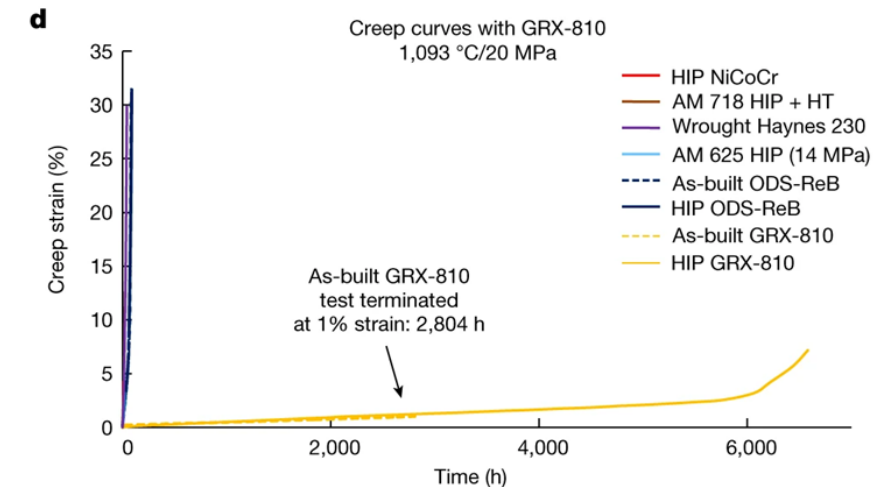
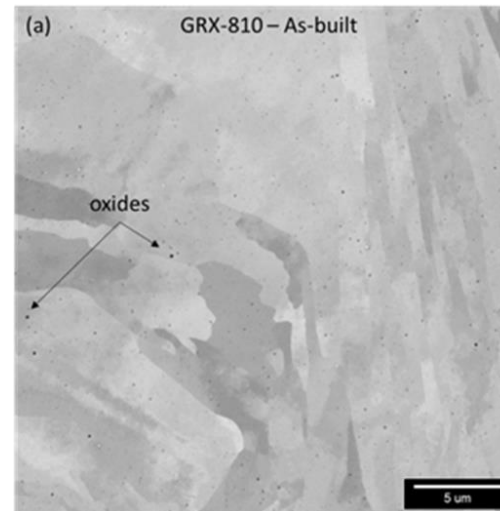
- GRX-810 alloy
- Atomistic modeling techniques
- Application to oxidation in pure Ni
- Extension to ODS alloys

Development of GRX-810 alloy at NASA



Alloy	Ni	Co	Cr	Re	Al	Ti	Nb	W	C
New composition (GRX-810)	Bal.	33	29	1.5	0.3	0.25	0.75	3.0	0.05

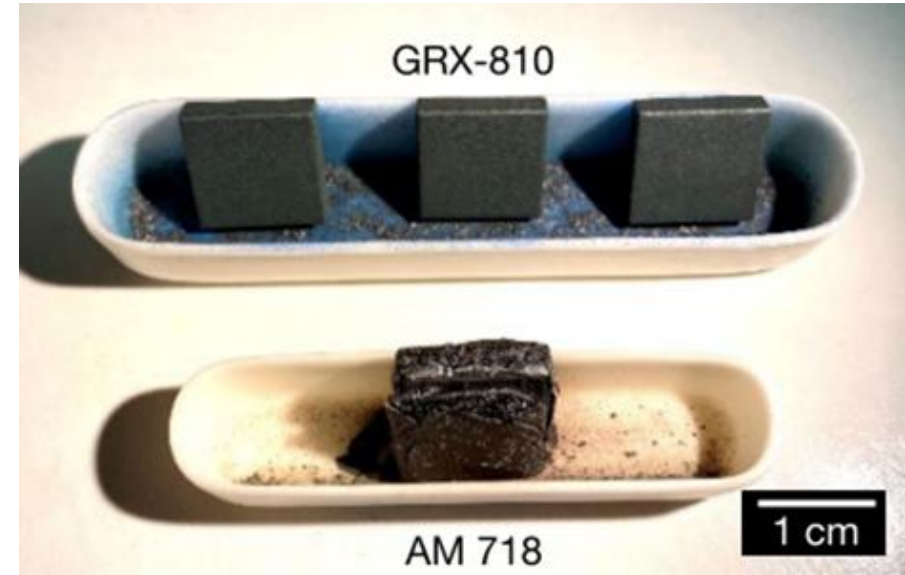
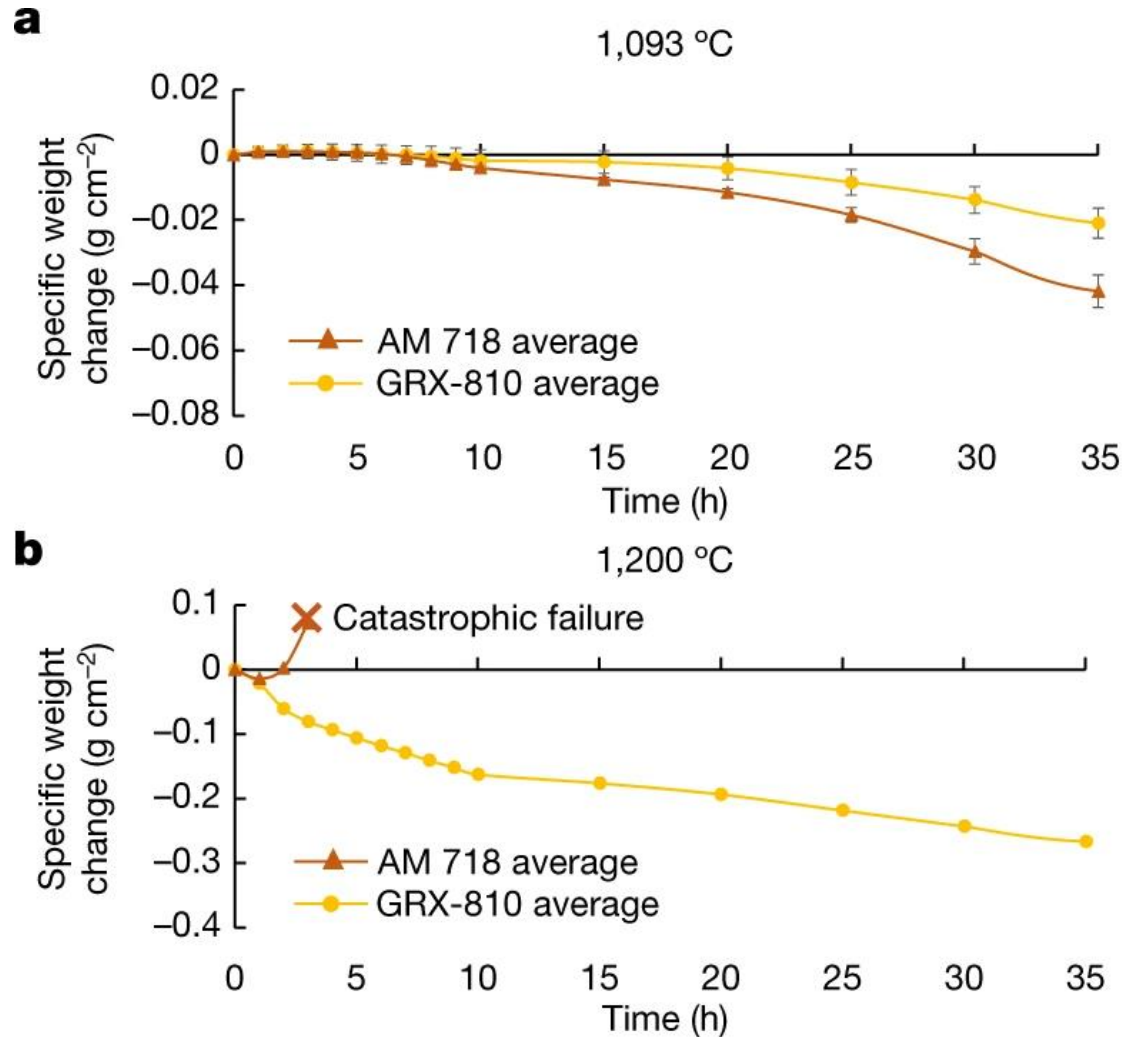
+ Y2O3



- GRX-810 is an alloy designed for the additive manufacturing of complex geometry engine components subjected to high temperatures.

- The matrix is an FCC medium entropy alloy with oxide dispersion strengthening.
- It has attracted significant attention due to its unprecedented high temperature creep properties.

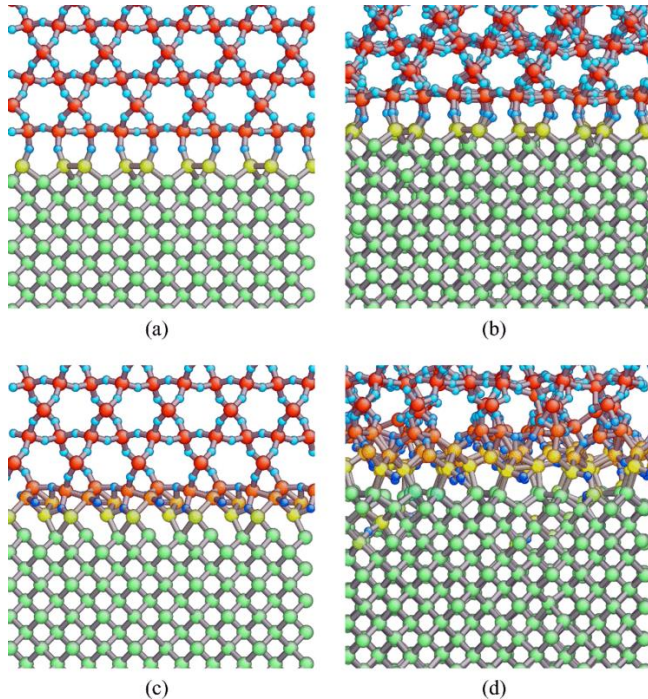
GRX-810 oxidation resistance



- GRX-810 outperforms other chromia-forming alloys in high temperature cyclic oxidation.
- Improved scale adherence hypothesized to be a result of Y_2O_3 additions – reactive element effect.

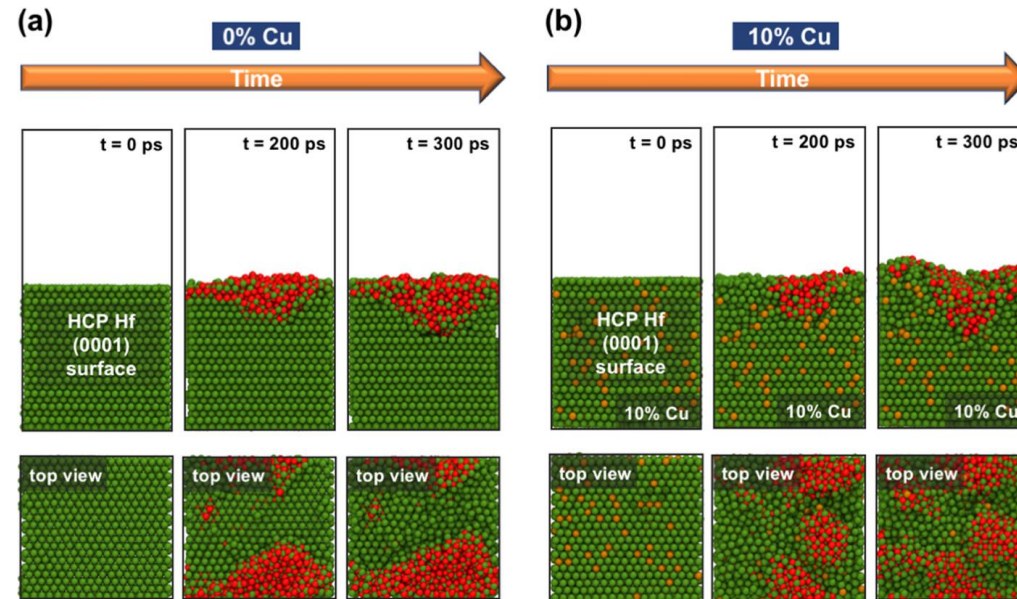
Atomistic simulations can provide key insights

Determination of interfacial structures



Lee et al., *Phys. Rev. B* 93, 144110 (2016)

Simulation of atomic-scale mechanisms



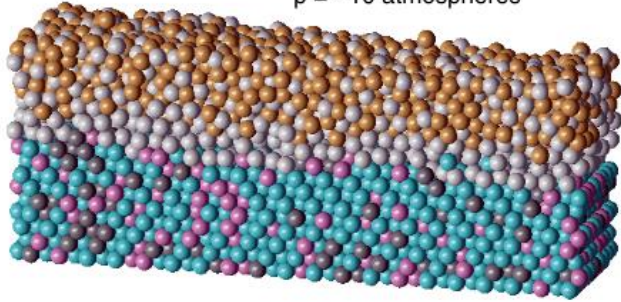
Sasikumar et al., *Chem. Mater.* 31, 3089 (2019)

- Molecular dynamics (MD) simulations of metal-oxide systems require specialized interatomic potentials to accurately describe the heterogeneous bonding – **typically expensive, limiting the scale of simulations.**

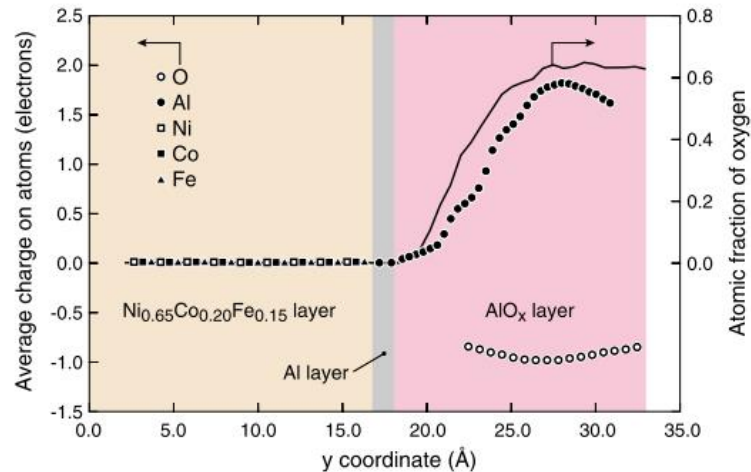
Variable charge MD simulations

(b)

Atomic oxygen pressure:
 $p \approx 10$ atmospheres



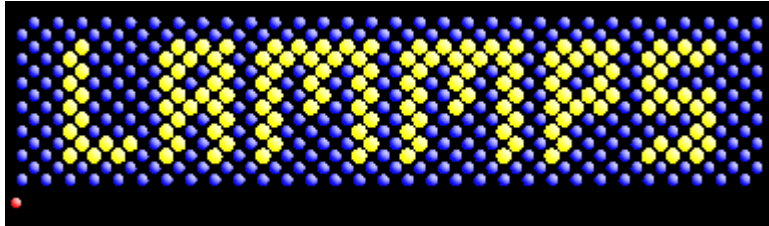
(c)



- Stages in each variable charge MD step:
 1. Obtain equilibrium atomic charges based on an energy minimization algorithm.
 2. Get atomic forces based on interatomic potential.
 3. Advance atomic positions.
- Step 1 traditionally makes variable charge MD expensive – we have introduced several efficiency improvements enabling improved scaling.

- Change from ionic to metallic bonding requires a variable charge scheme

New LAMMPS implementation



docs.lammps.org
pair_style coul/ctip
fix qeq/ctip

The Journal
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ARTICLE

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Development of interatomic potential suitable for molecular dynamics simulation of Ni oxidation and Ni-NiO interface

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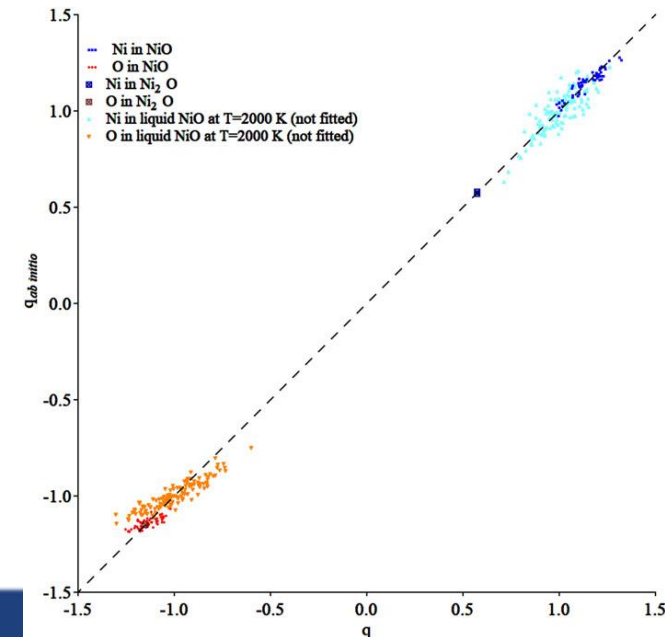
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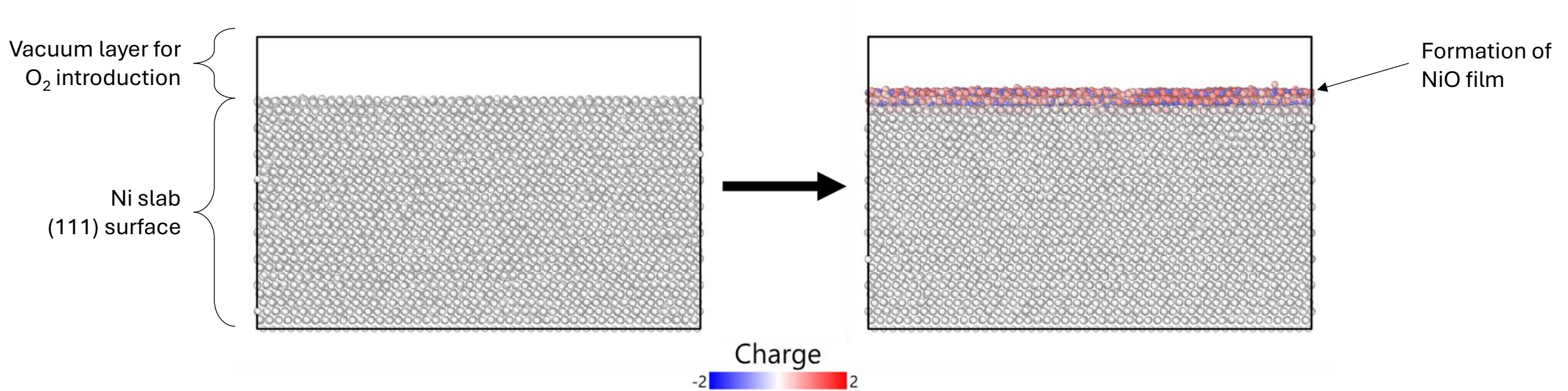


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- Introduced improvements:
 - Efficient evaluation of Coulomb interactions (linear scaling)
 - Partitioning of system into charged and uncharged regions
 - Optimized parallelization
- The new implementation can be coupled with any type of potential – classical, machine learning

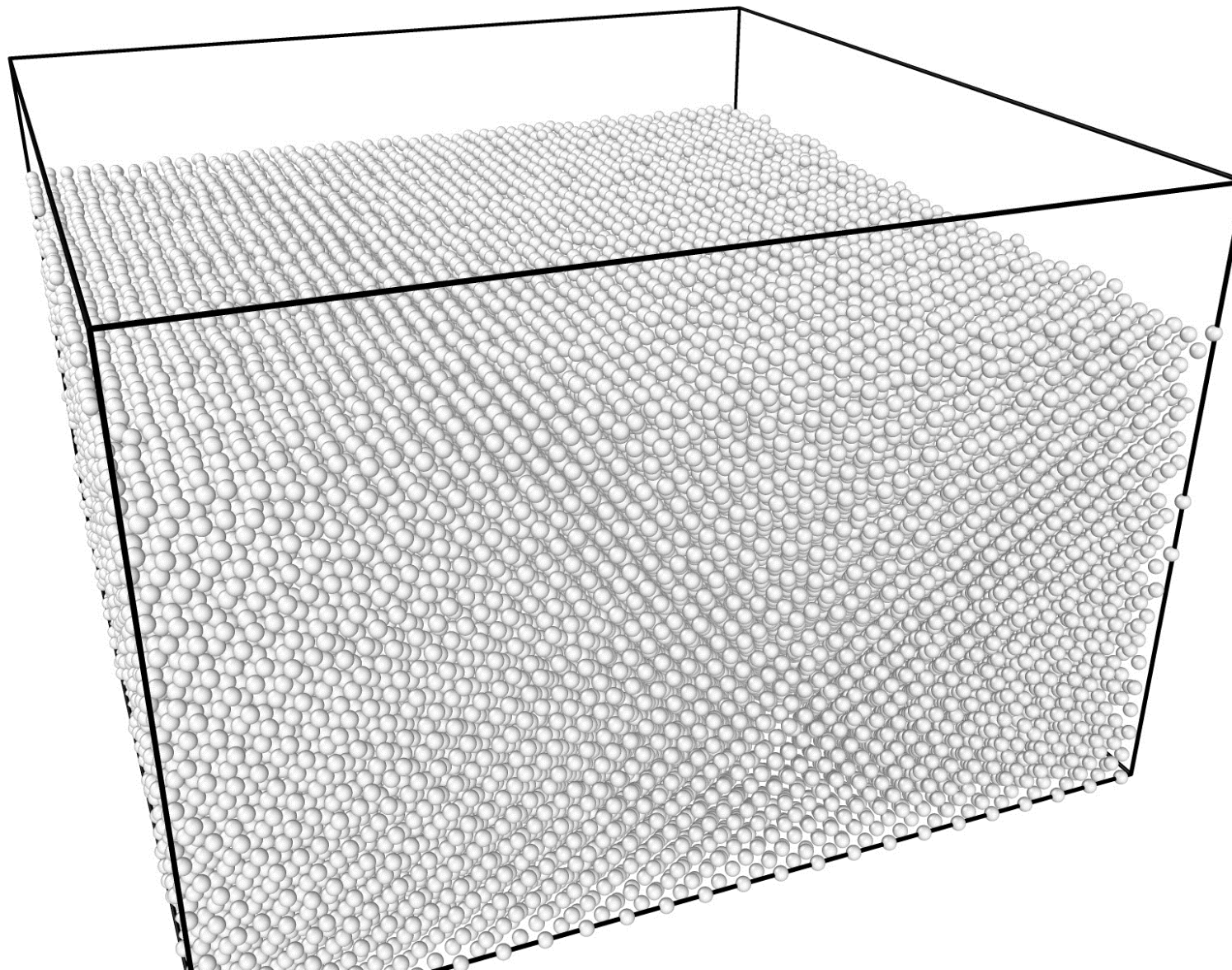


Simulating Ni oxidation

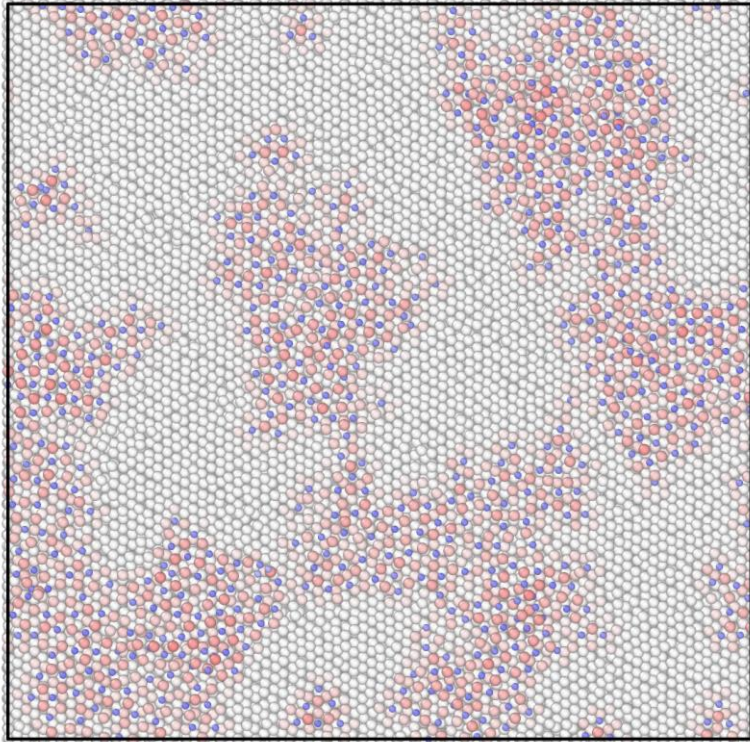


- ~50,000 atoms – ~**5x** more than prior work.
- 20-30 ns simulation time - ~**100x** longer than prior work.
- These scales were necessary to observe the relevant mechanisms.

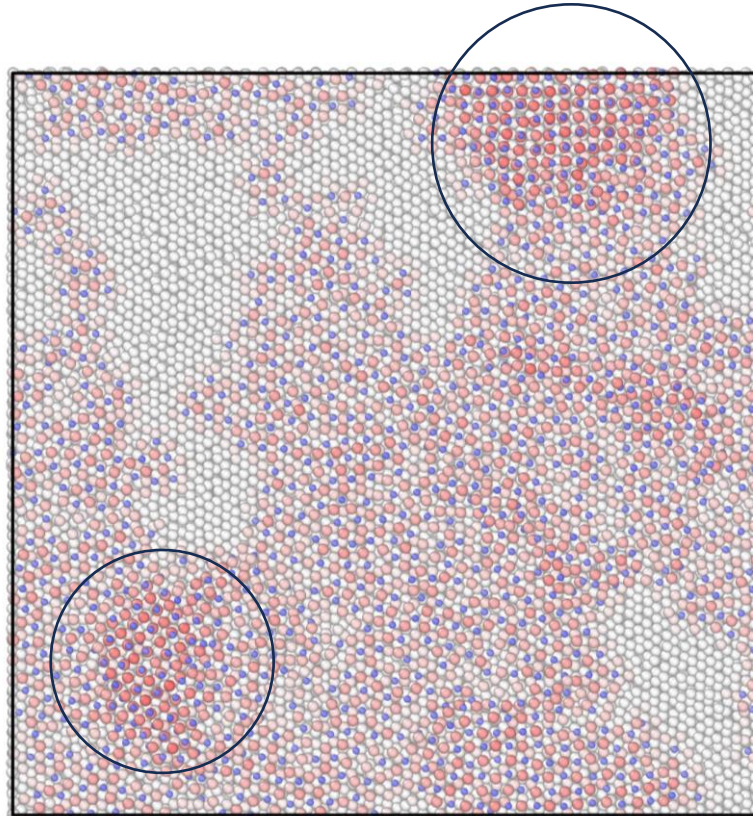
Oxidation at 800 K



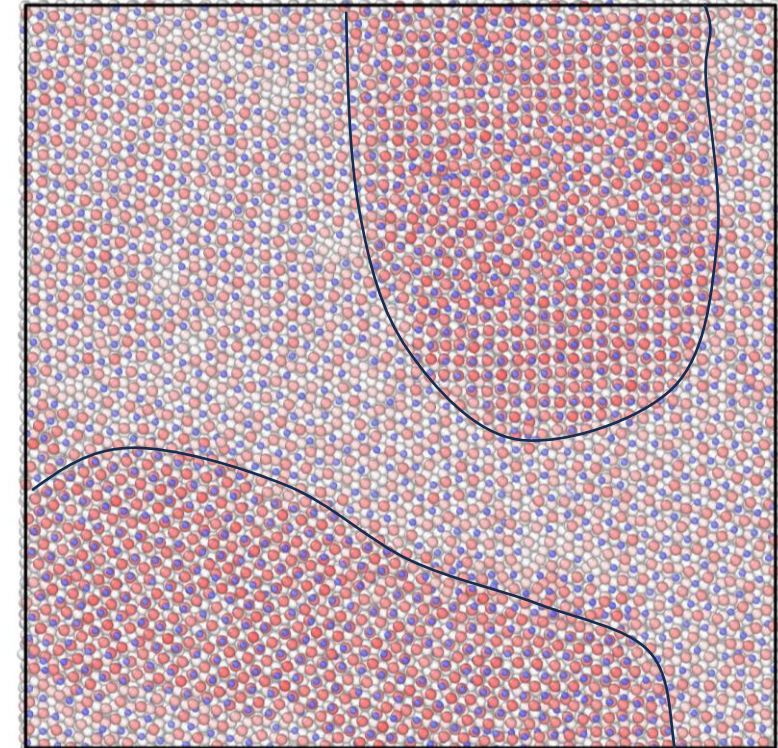
Mechanisms of oxide film formation



Initial stage of
dissociation and
adsorption

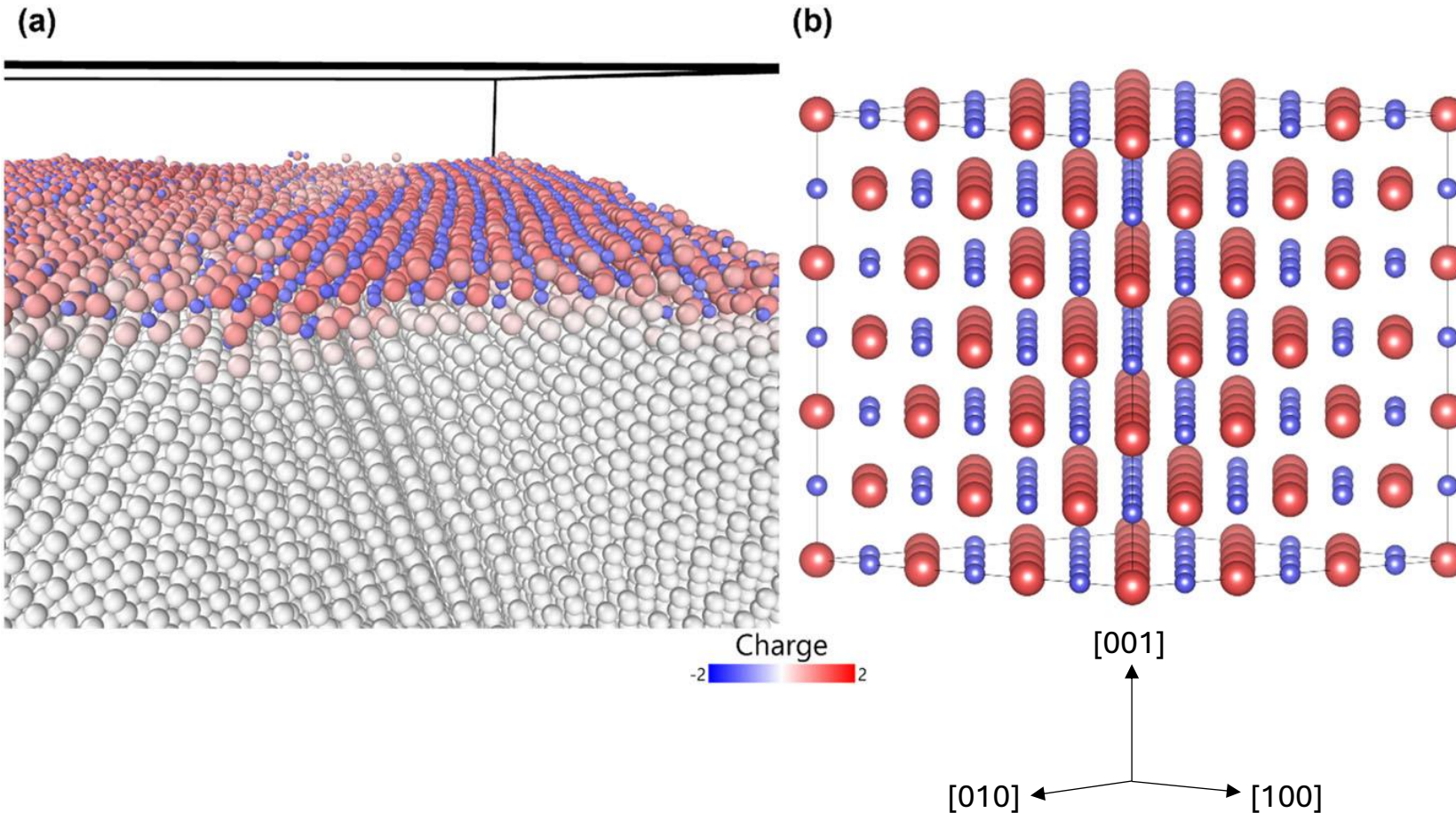


Nucleation of ordered
oxide regions



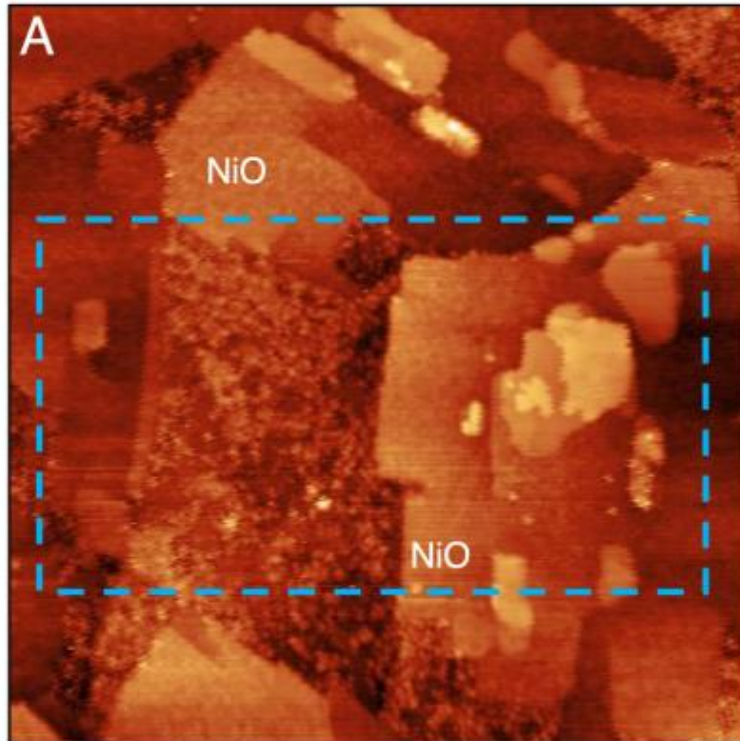
Planar growth of oxide
across surface

Structure of the oxide film



- NiO film crystallizes in the correct B1 (rock salt) structure.
- The non-polar (100) surface is exposed.
- Prior MD simulations of oxidation could not observe this mechanism due to length and time scale limitations.

Simulation has excellent agreement with experiment



- STM imaging confirms the formation of planar NiO domains with the same Ni(111)-NiO(100) interface

Stage 1

Cr-oxide particles

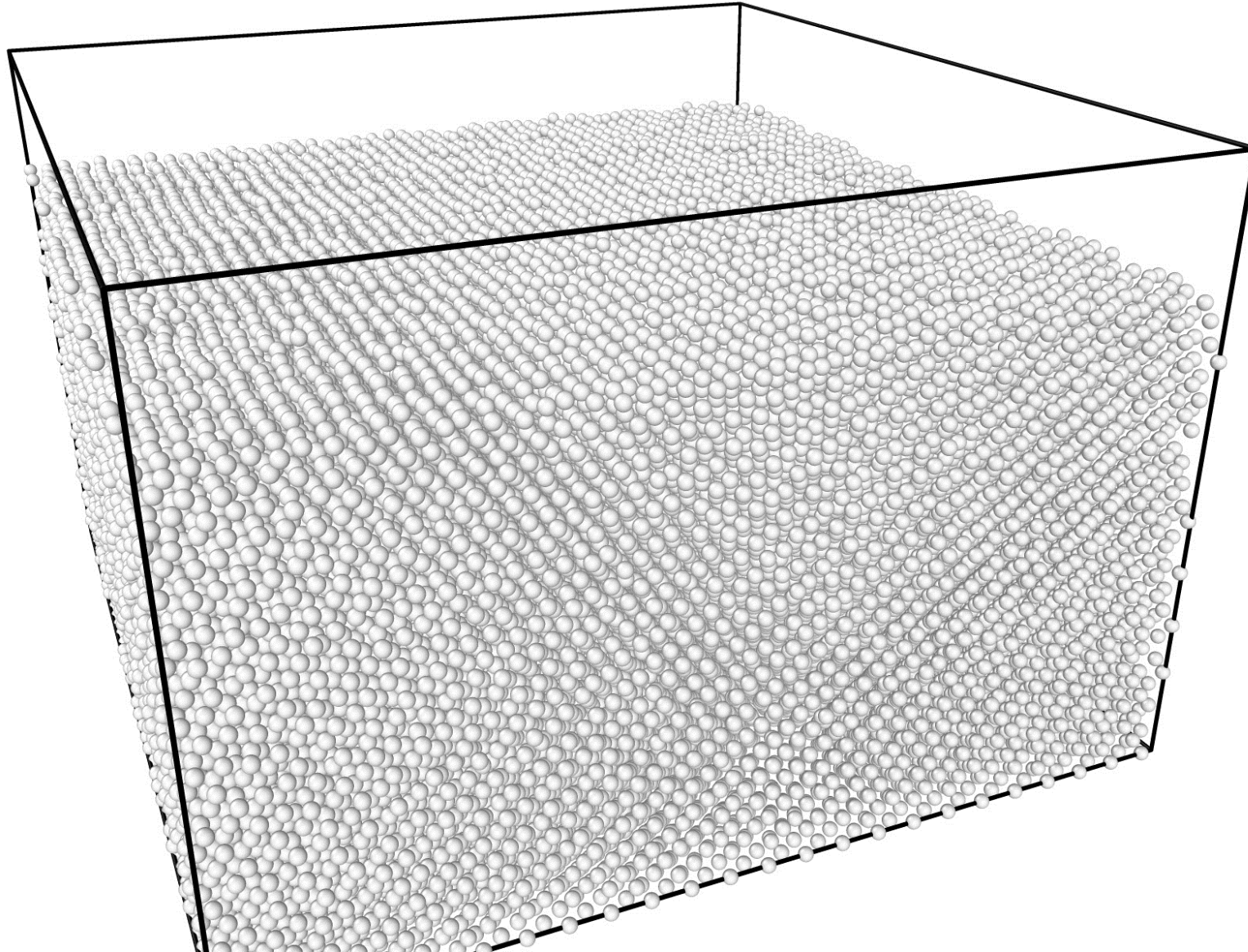
Cr-rich oxide particles preferentially nucleate on both the terraces and step edges

NiO

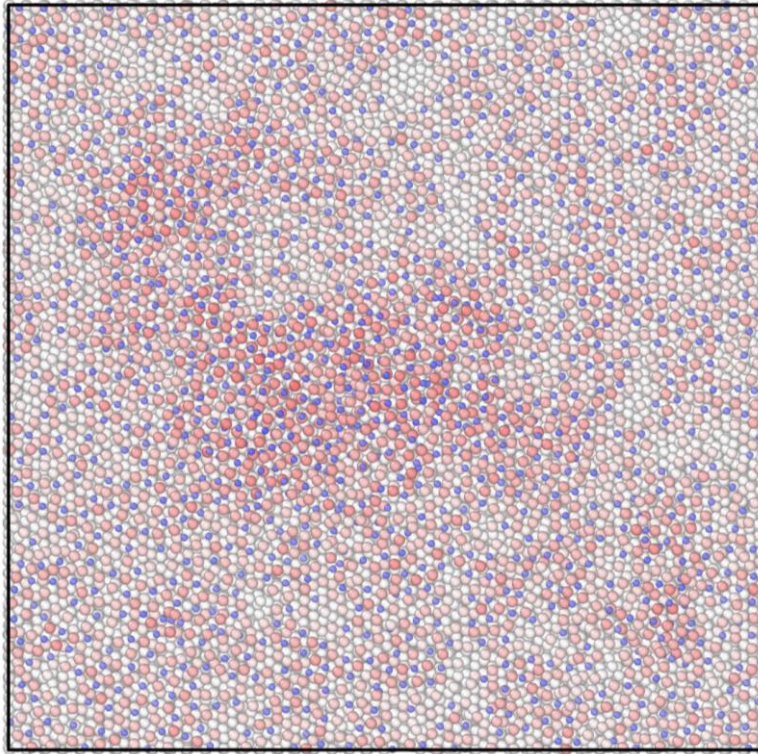
2D layers of NiO(100) nucleate and grow across terraces, pinned between step edges and particles



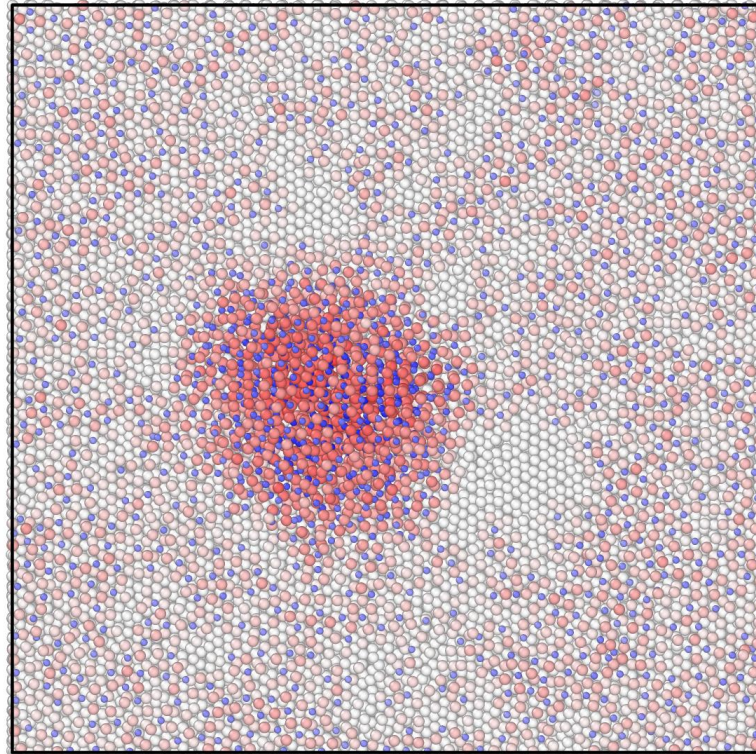
Increasing temperature to 1000 K



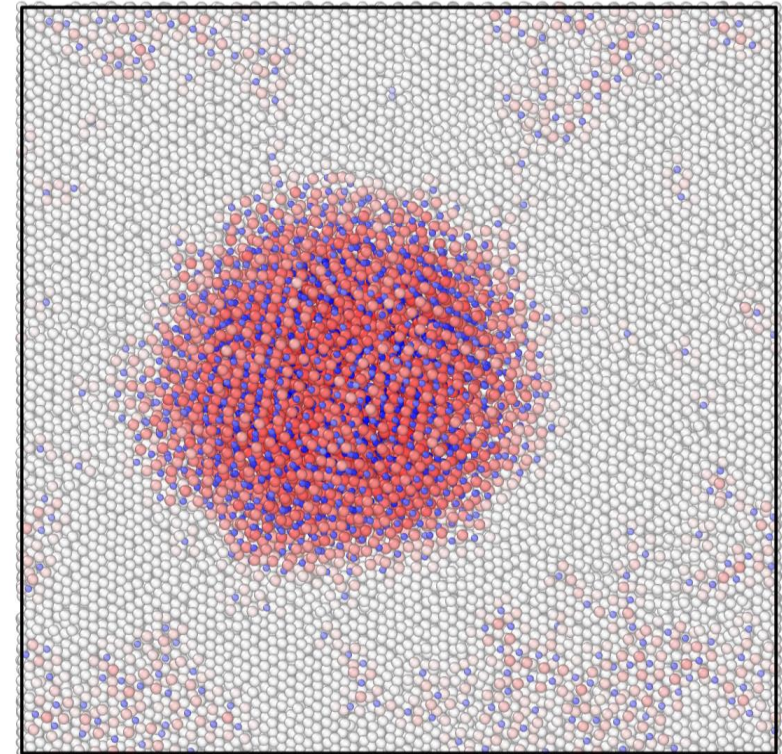
New mechanism activated



Initial stage of
dissociation and
adsorption



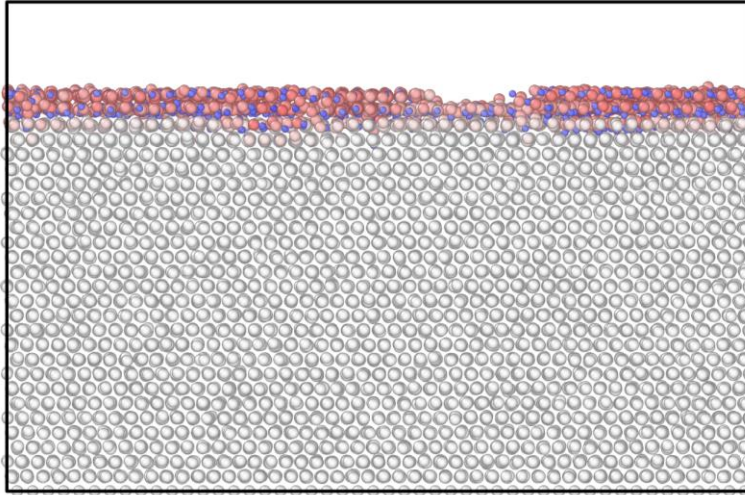
Nucleation of large oxide
island



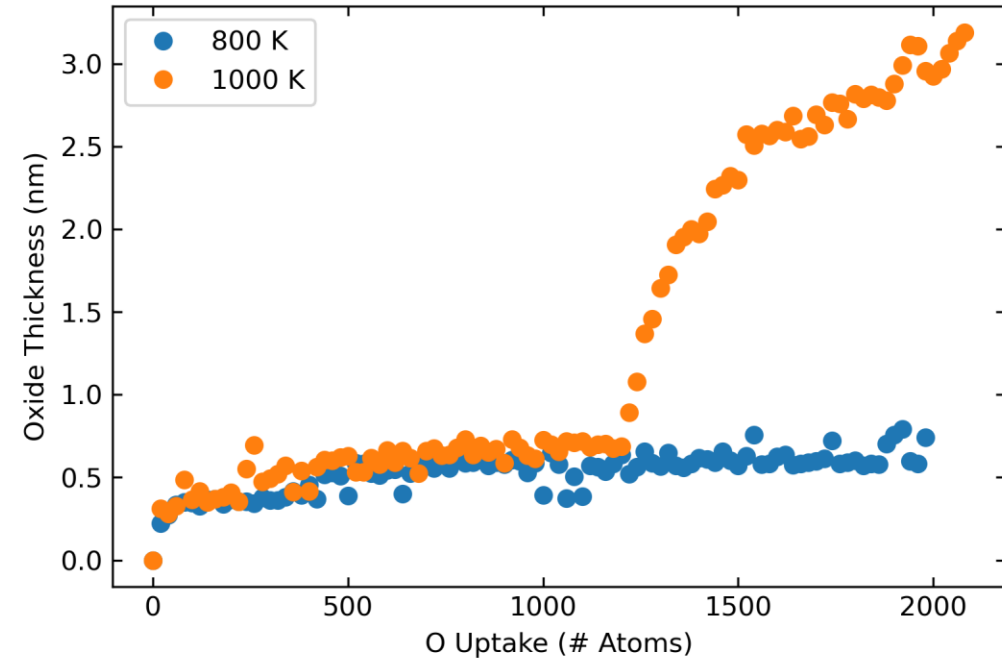
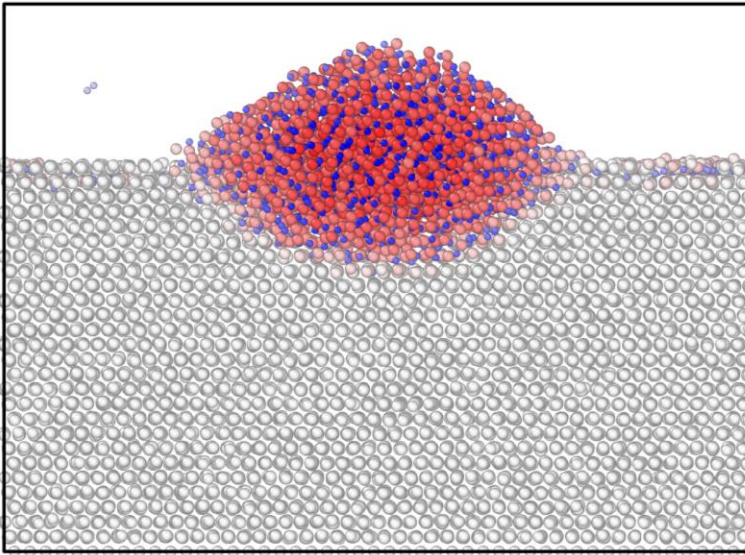
Lateral and vertical
growth of oxide island

New mechanism allows for accelerated oxide growth

800 K



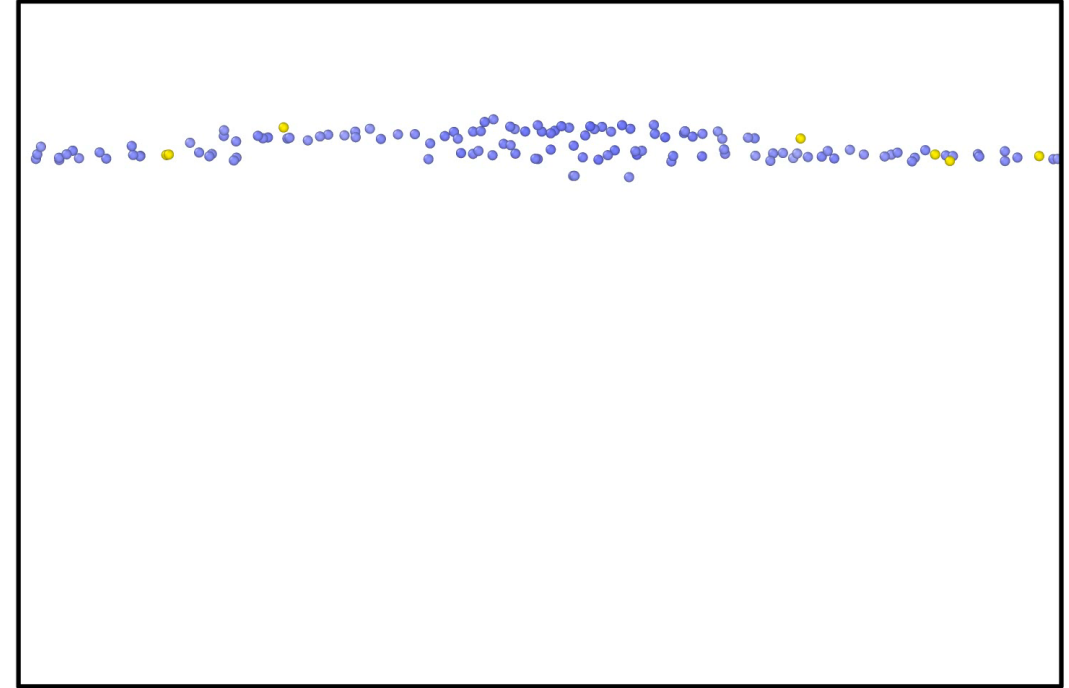
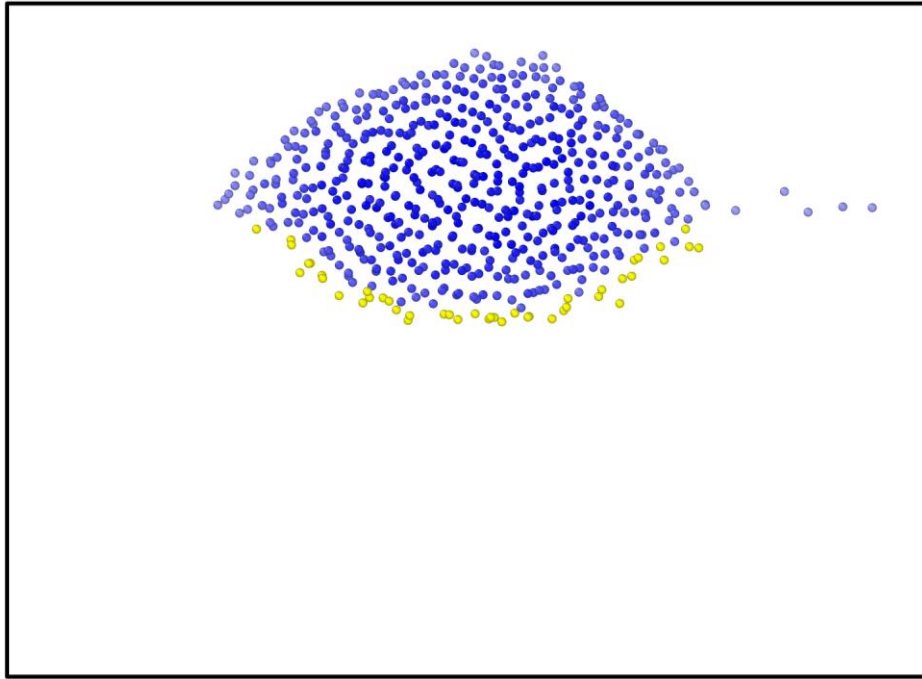
1000 K



- O atoms diffuse more easily into the bulk Ni.
- Kinetic changes can be linked to atomic scale mechanisms with simulations.

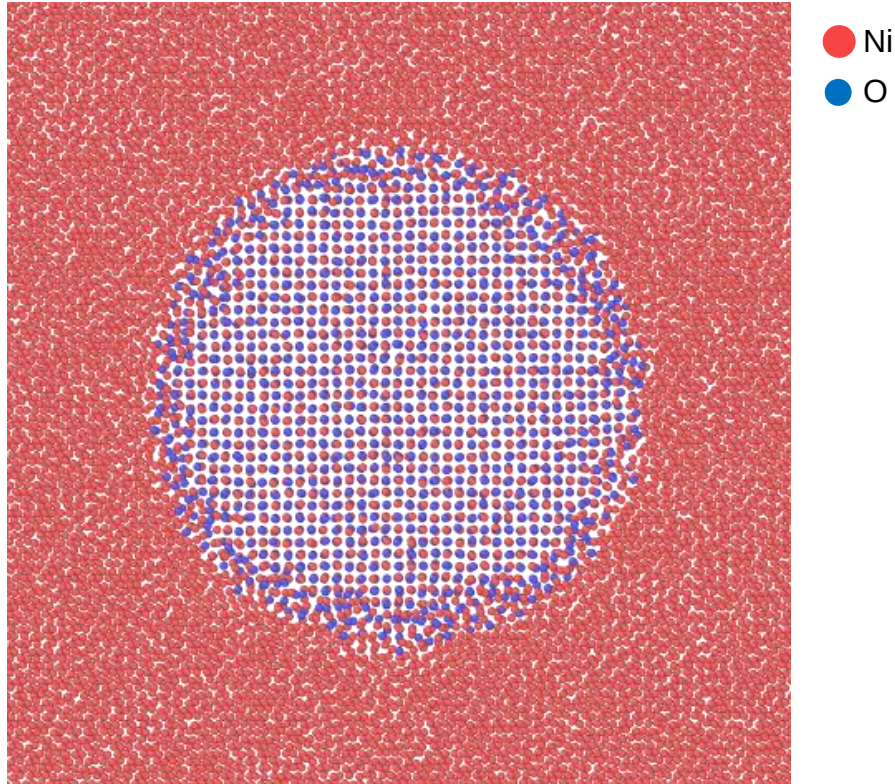
Ni-NiO interface provides an easy diffusion pathway at high temperatures

*Only O atoms shown



- Diffusion at these rates implies a liquid-like interfacial region.

Extensions to ODS alloys



- Newly developed simulation methods can accurately model oxide particles embedded in a metal matrix.
- How will the presence of Y₂O₃ particles affect oxidation mechanisms and kinetics?
- Enabling atomistic investigations of the reactive element effect:
 - Oxide film adherence
 - O transport
- New insights into optimization of oxidation resistance.

Summary and acknowledgements

- GRX-810 is an additively manufactured ODS alloy with unprecedented high temperature properties, including creep and oxidation resistance.
- New methods in atomistic simulations can provide insights into the underlying mechanisms governing such properties.
- How can we use these tools to better understand and design for oxidation resistance?

