Effects of Cr twinning in Ni-based superalloys

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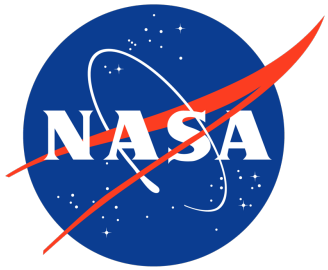
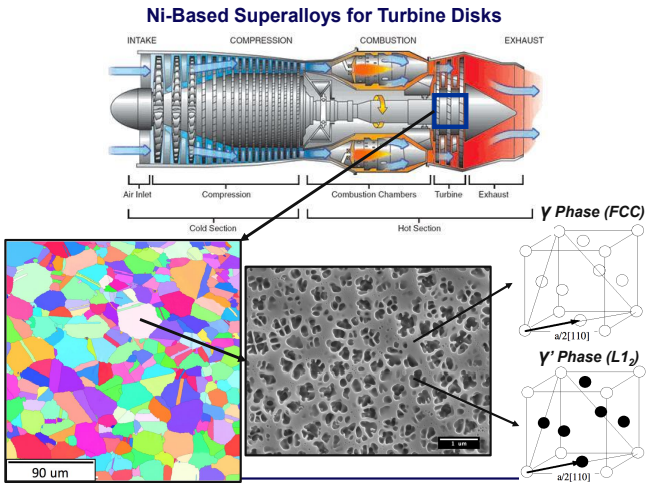
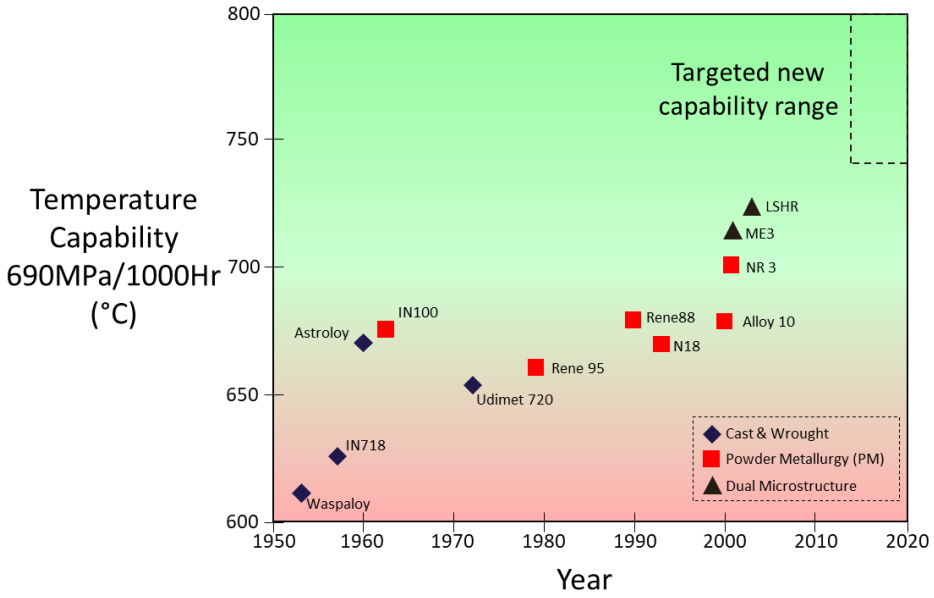


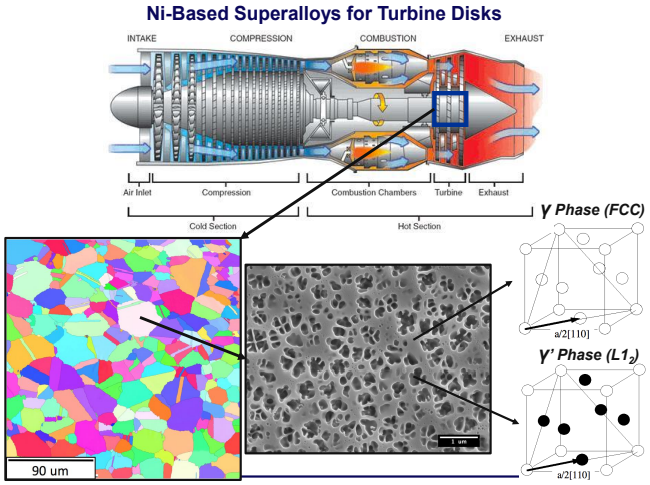
Progress in turbine disk alloys

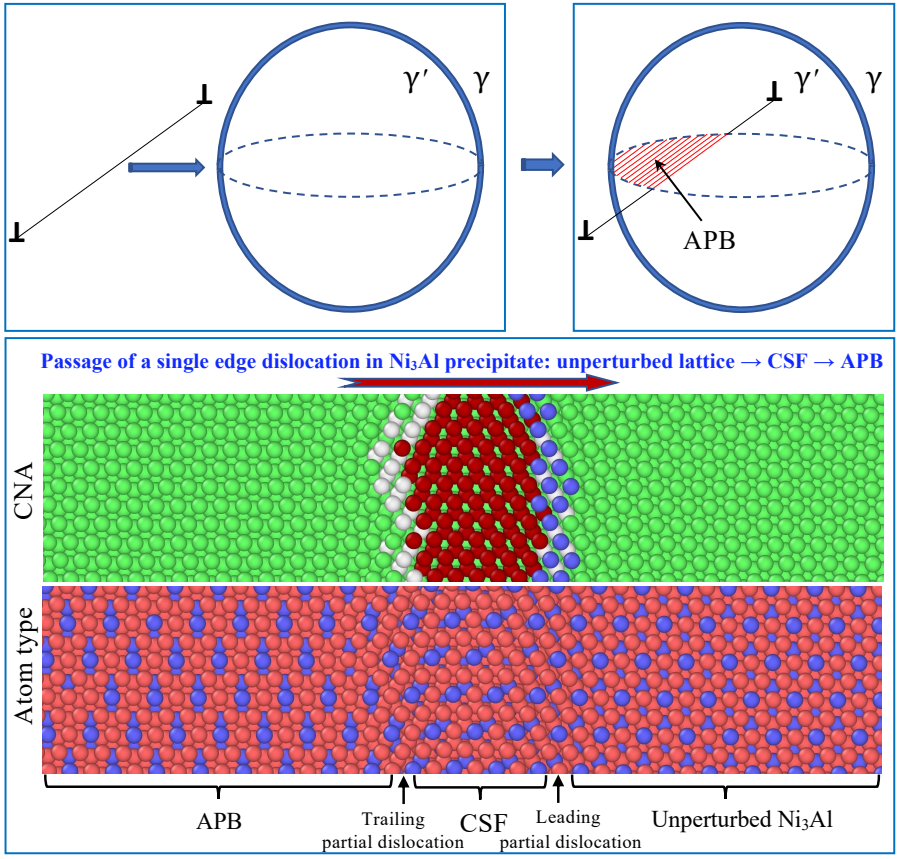




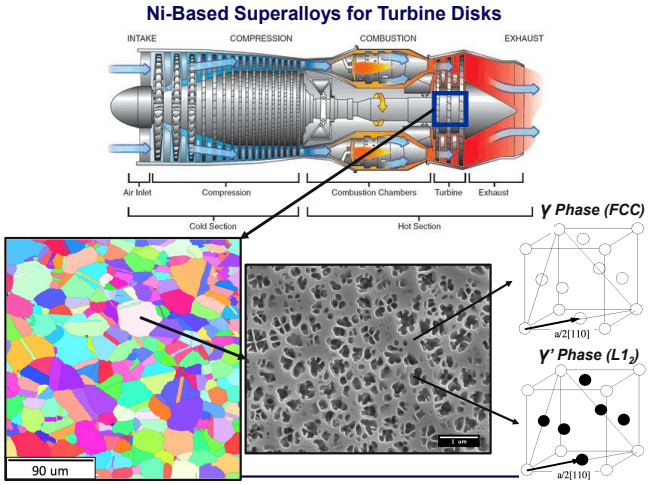
- Increase of the operating temperature of turbine engines is required to improve the efficiency and reduce the emissions.
- New deformation mechanisms (thermally activated) become important above 700 °C.
- Understanding the effects of microstructure and composition on functionality of these creep deformation mechanisms will lead to design of new materials with improved creep resistance.

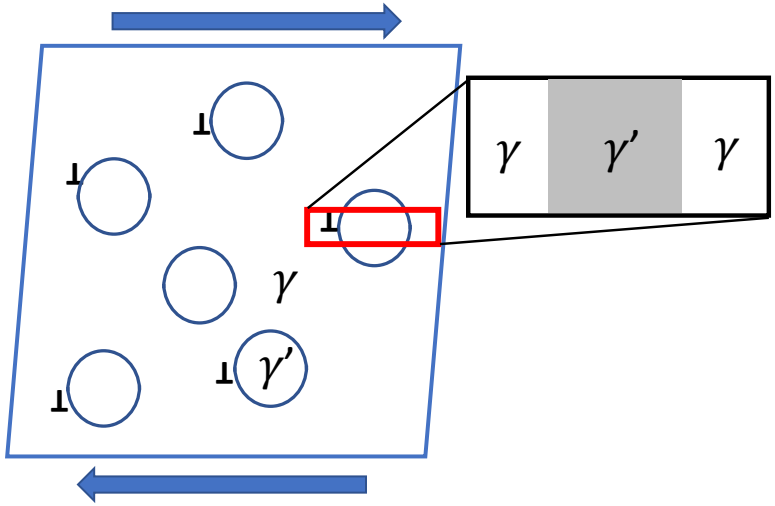
Deformation mechanisms in Ni-based superalloys



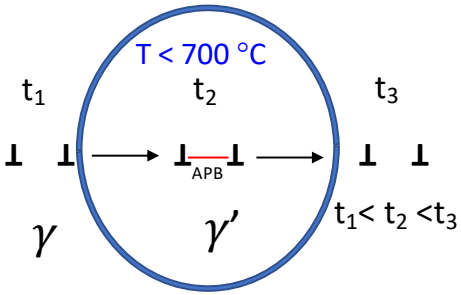


Deformation mechanisms in Ni-based superalloys

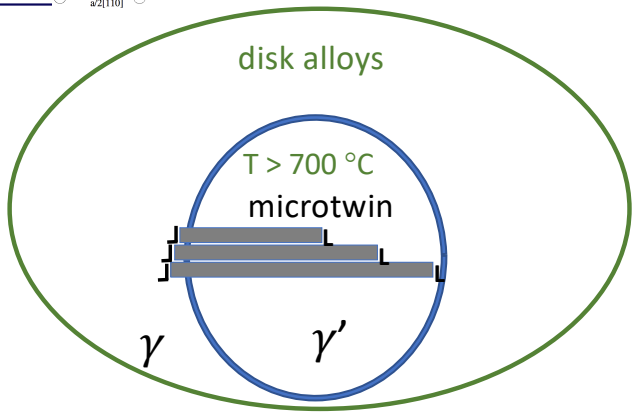




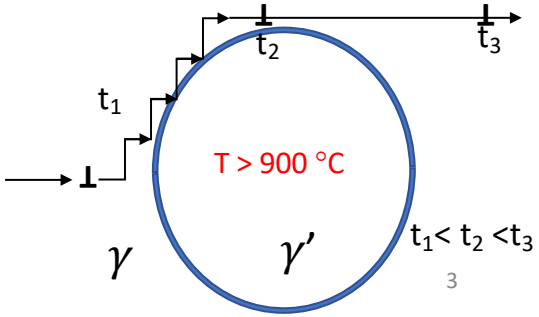
disk alloys



disk alloys



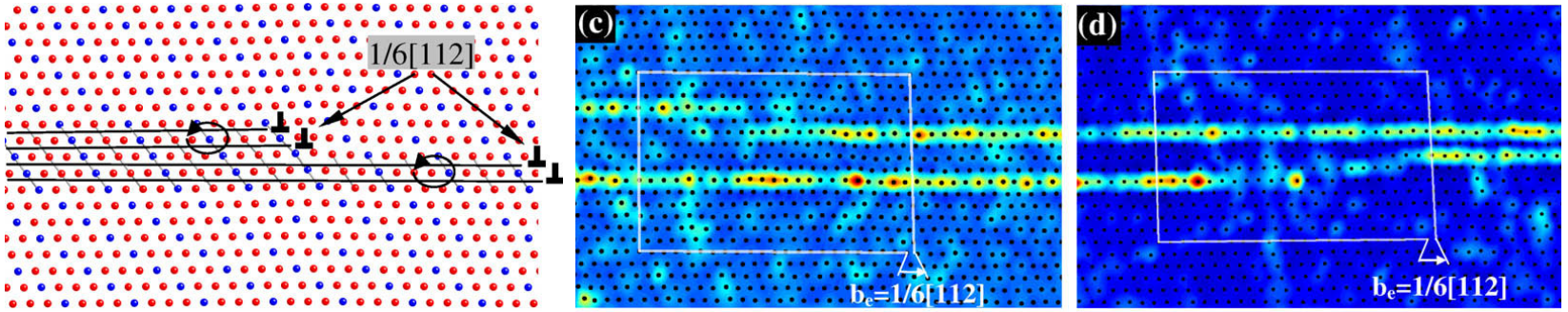
blade alloys



The Kolbe mechanism for micro-twinning

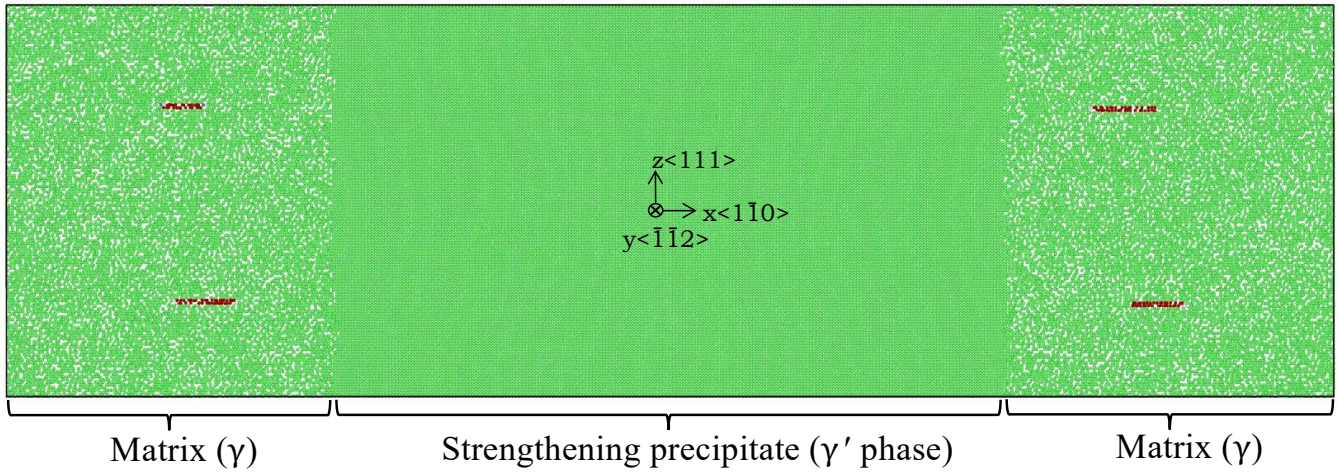
- Micro-twinning is a major creep deformation mechanism in Ni-based superalloys at intermediate temperatures.
- Many aspects of twin nucleation and growth remain unexplored.
- The Kolbe mechanism for micro-twinning, based on thermally activated reordering, is currently widely accepted in the community to explain these processes.

Kovarik *et al.*, PMS 2009



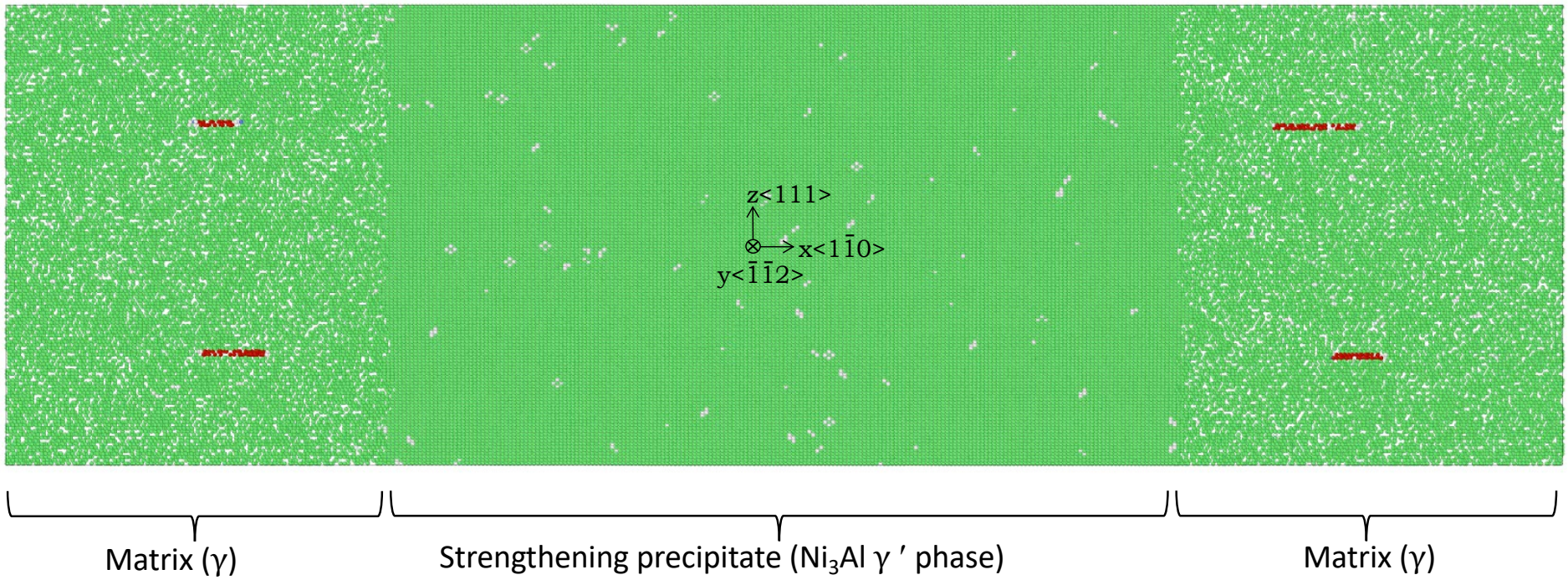
Simulation geometry and procedure

- Composite simulation system (Ni-Al), containing γ phase (matrix) and γ′ phase (precipitate) regions and two edge dislocation dipoles.
- LAMMPS package; Ni-Al interatomic potential by Mendelev.
- Simulation cell size: ~100×2.5×30 nm^3 (~7×10^5 atoms). PBCs in all directions.
- 350 vacancies introduced in the system to simulate diffusion mediated reordering.
- The system was equilibrated at T = 1300K, using hybrid MC/MD prior to introduction of dipoles.
- The dipoles were positioned in such a way that individual dislocations of upper and lower dislocation pairs would glide on adjacent {111} planes when a shear stress was applied.

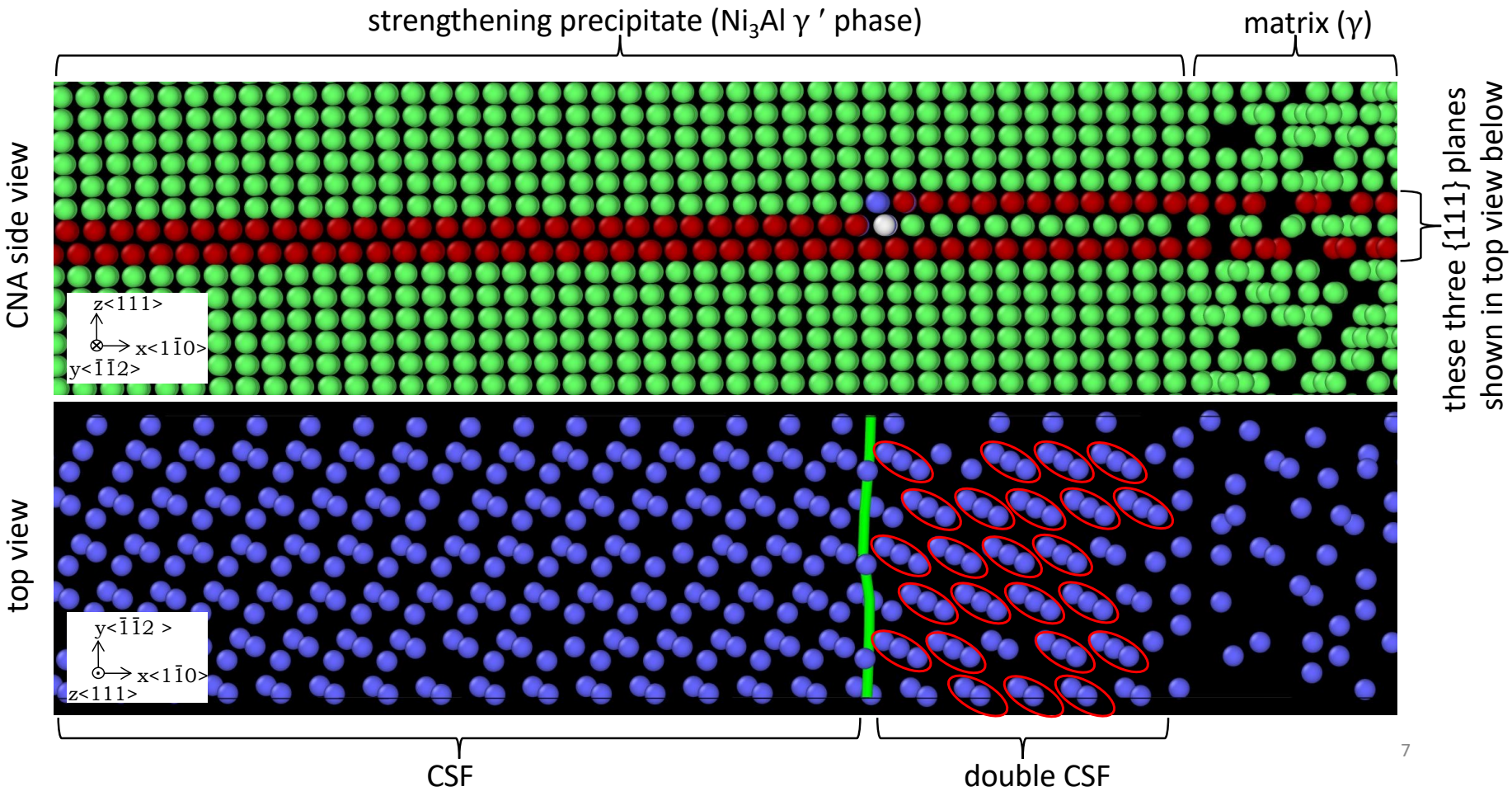


The Kolbe mechanism for micro-twinning

potential for NiAl by Mendelev; NPT, T=1300K; 350 vacancies; σ_{xz}= 600 Mpa, σ_{yz}= 1039 Mpa; Ni atoms not shown



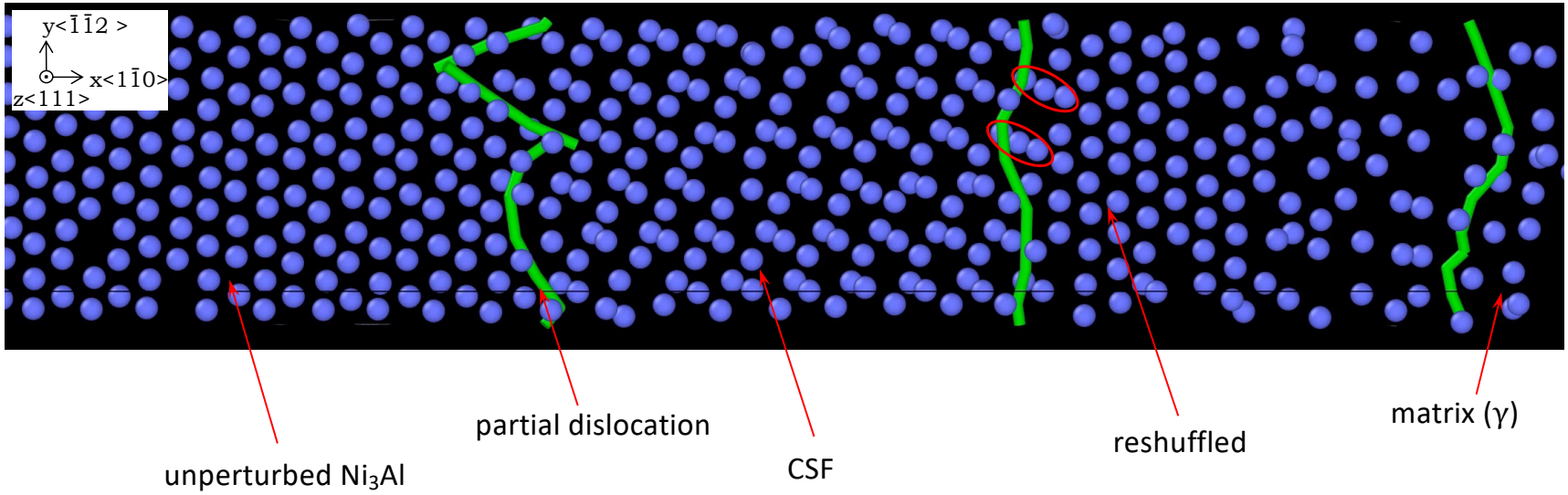
The Kolbe mechanism for micro-twinning



The Kolbe mechanism for micro-twinning

Dislocations (green); **Al** atoms (blue); high energy (red); Ni not shown

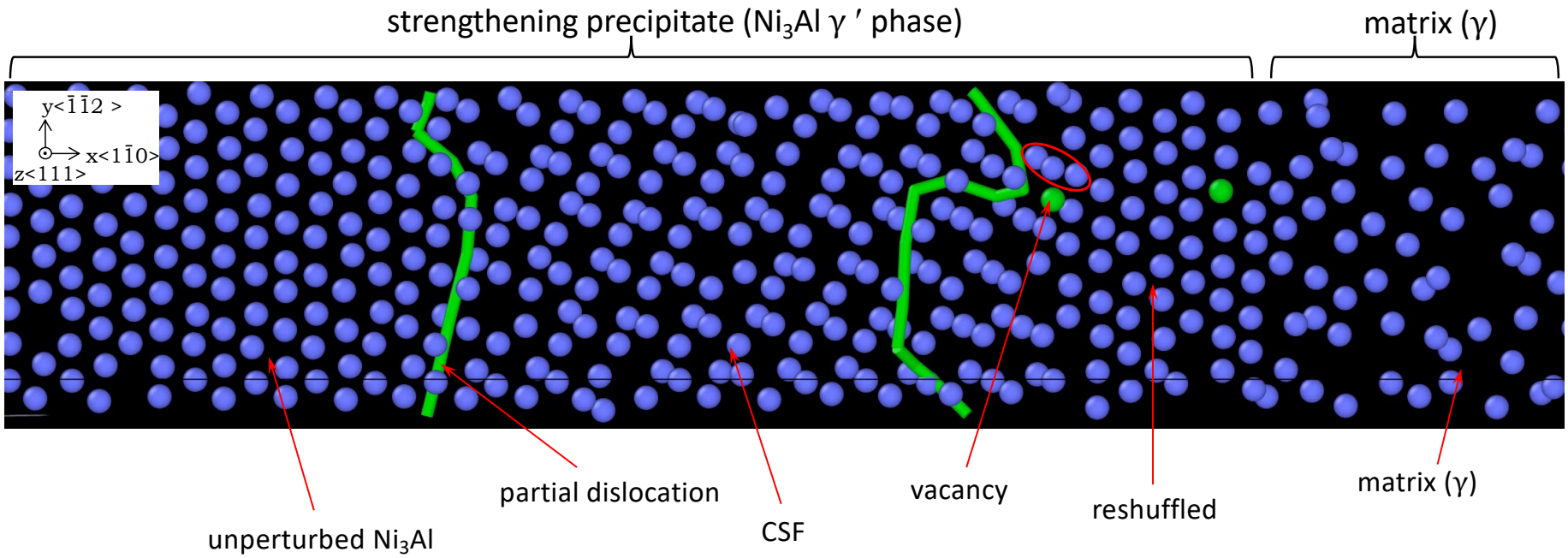
~ 0.1 μs of MD deformation run (350 vacancies, T=1300K, σ_{xz} = 600 MPa σ_{yz} = 1039 Mpa σ_{total} = 1.2 GPa)



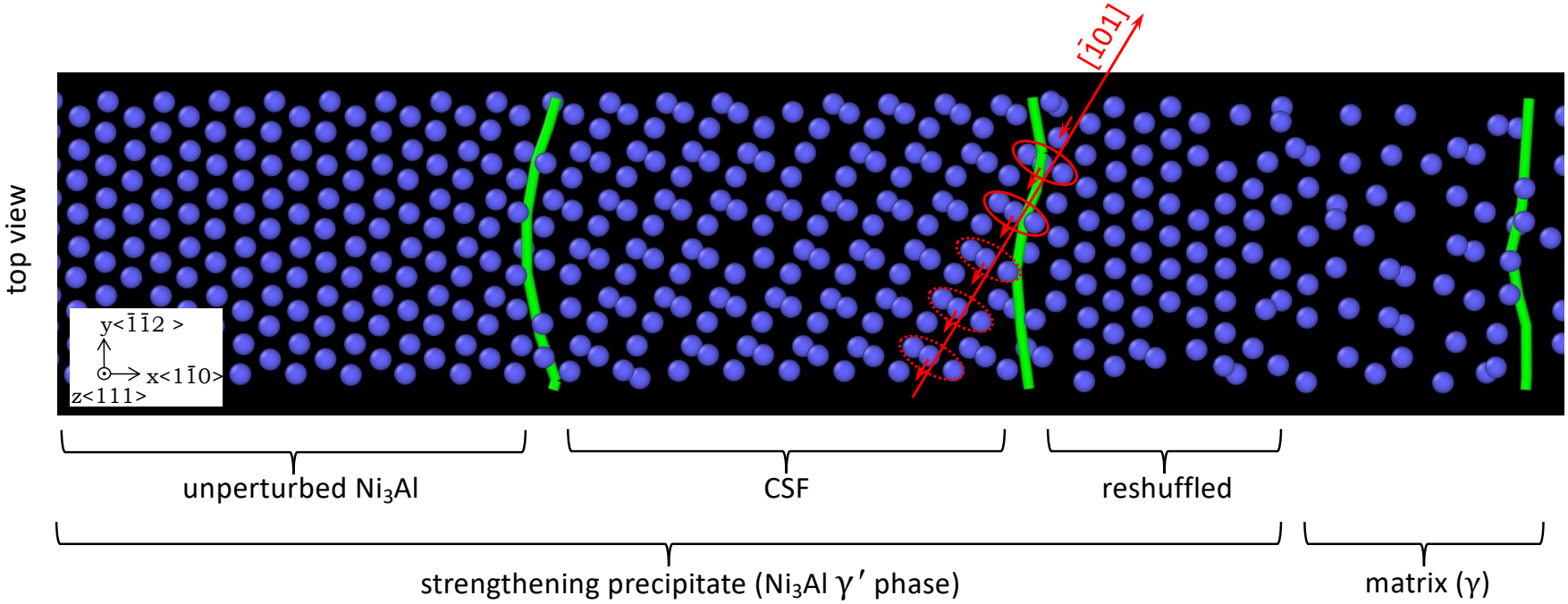
- Under applied stress, dislocations slowly move inside the precipitate. The reshuffling process (double CSF -> $L1_2$) is the major factor, determining the the speed of the propagation.

The Kolbe mechanism for micro-twinning: single reshuffling move

Single reshuffling move assisted by partial (vacancies are shown, Ni not shown)



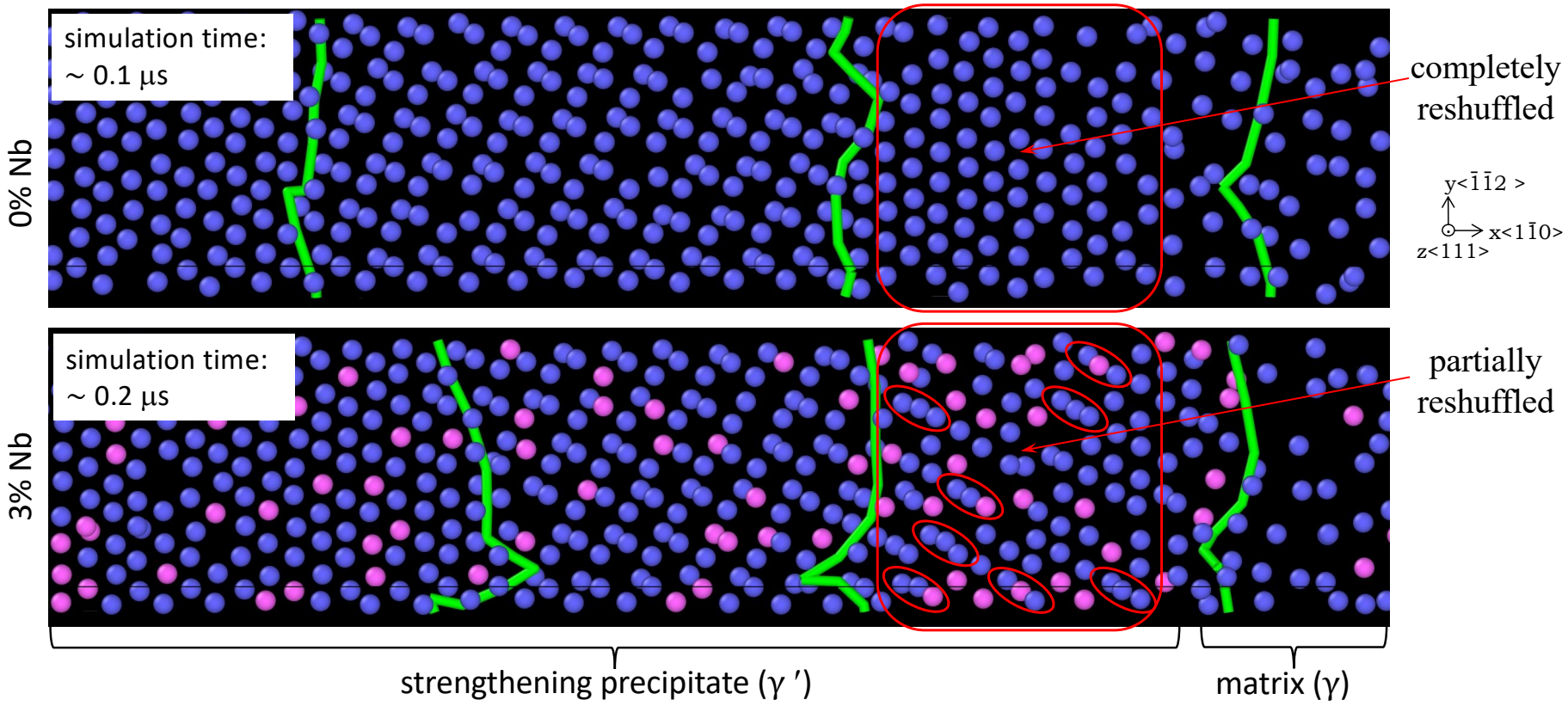
The Kolbe mechanism for micro-twinning



Borovikov, V. V., Mendelev, M. I., Smith, T. M., & Lawson, J. W. (2023).
"Dislocation-assisted diffusion-mediated atomic reshuffling in the Kolbe mechanism for micro-twinning in Ni-based superalloys from molecular dynamics simulation".
Scripta Materialia, *232*, 115475.

Effect of Nb on the Kolbe mechanism for micro-twinning

potential for Ni-Al-Nb by Mendelev; dislocations (green); Ni atoms are not shown



- Nb atoms suppress reordering, reducing deformation creep

Segregation of Cr at stacking faults in γ‘

Y. Rao et al. / Acta Materialia 148 (2018) 173–184

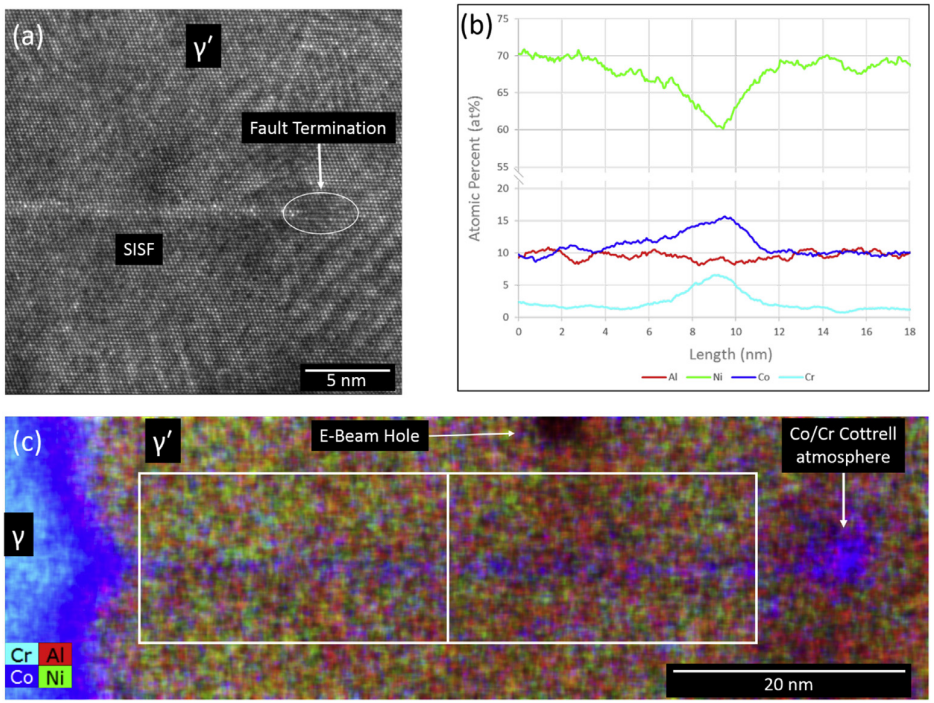
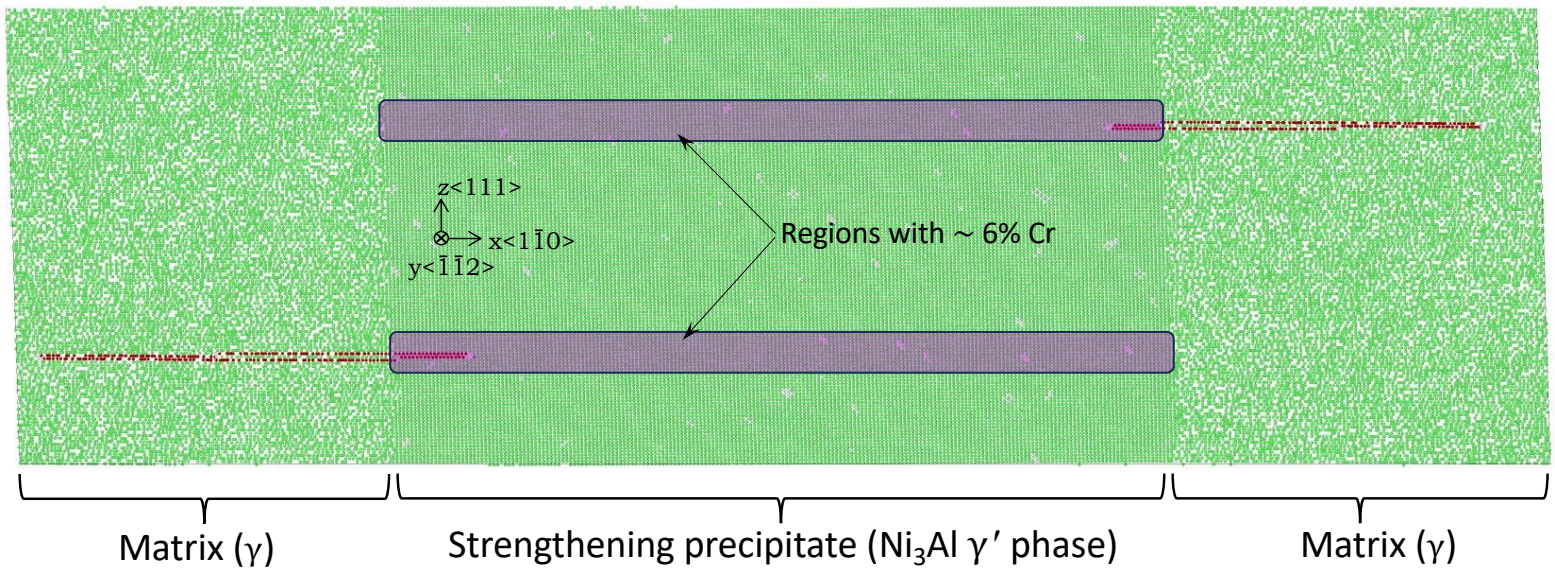


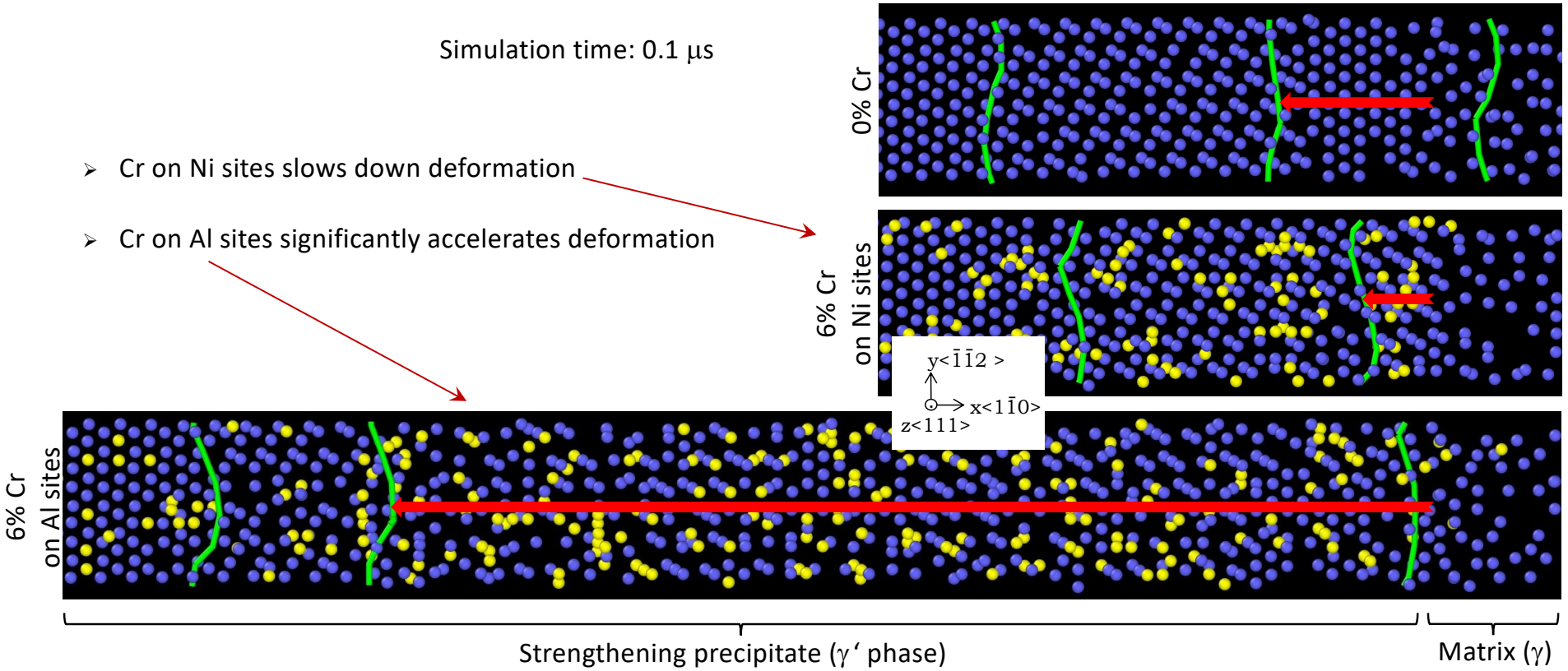
Fig. 5. (a) An atomic resolution HAADF image of a superlattice intrinsic stacking fault terminating inside a γ′ precipitate in the superalloy ME3. (b) An integrated line scan showing the element segregation across the SISF in (a). (c) Combined Cr, Co, Al, and Ni elemental maps of the entire SISF shown in (a). The white box represents the area integrated for the quantified line scans in (b). A notable Co and Cr-rich Cottrell atmosphere is observed around the shearing Shockley partials on the right side of the EDX map.

Modeling the effects of Cr on the Kolbe mechanism for micro-twinning

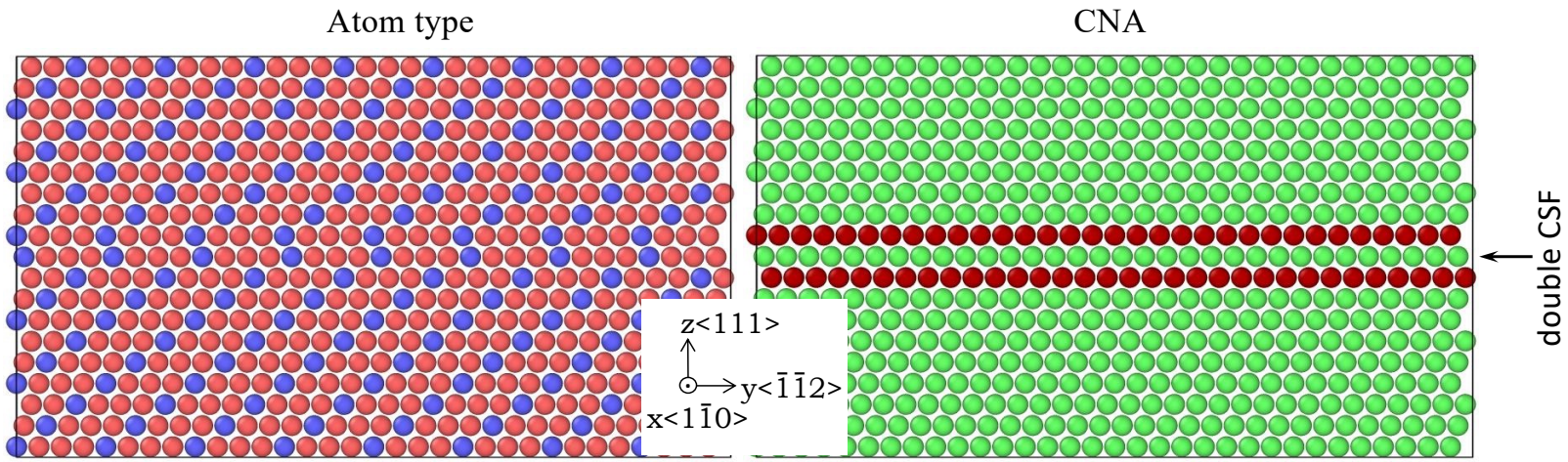


Effects of Cr on the Kolbe mechanism for micro-twinning

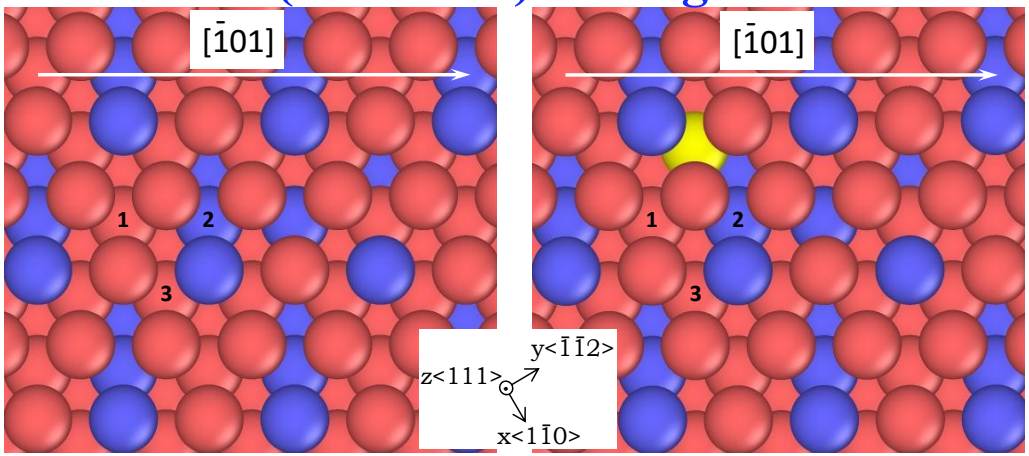
potential for Ni-Al-Cr by Mendelev; T=1300K; dislocations (green); Ni atoms are not shown

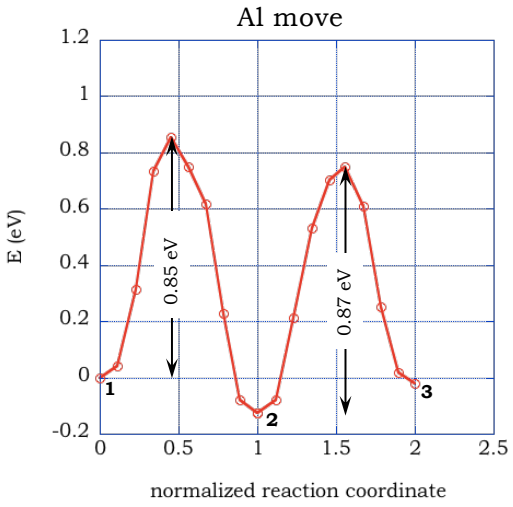


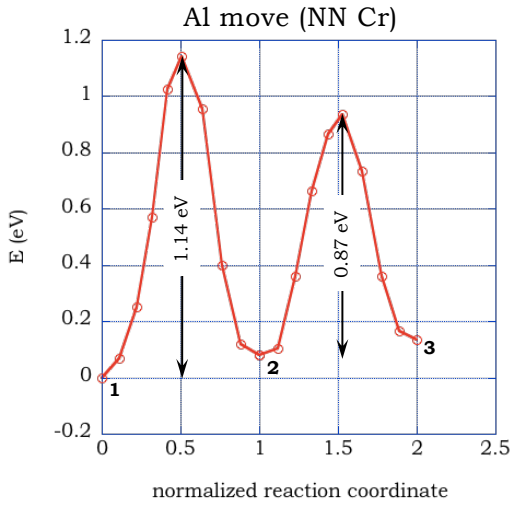
Effect of Cr (on Ni site) on migration barriers



Effect of Cr (on Ni site) on migration barriers







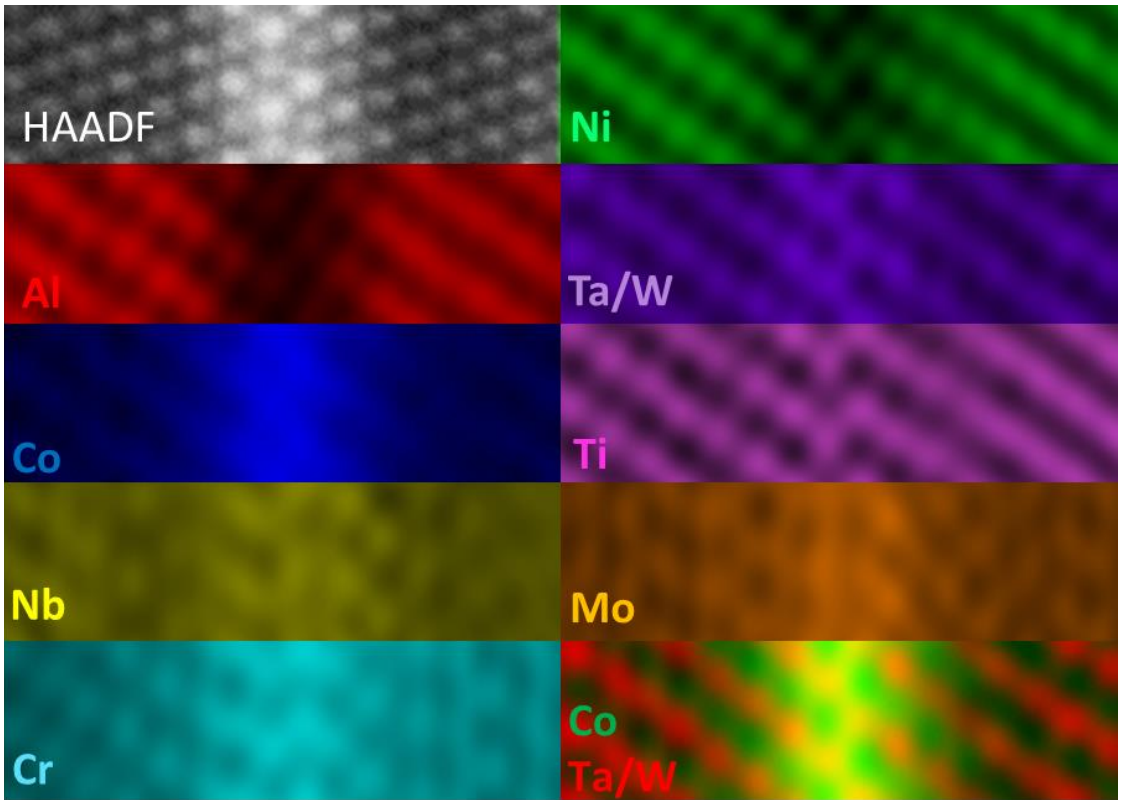
Experimental puzzle

A new disk superalloy was recently developed by NASA: NASA Alloy 1

Average alloy compositions in atomic percent

Alloy	Ni	Cr	Co	Al	Ti	Nb	Ta	Hf	Mo	W	Zr	Fe	B	C
NASA alloy 1	51.79476	12.60713	19.31268	6.452026	3.724641	0.943347	1.599034	0.124438	1.633071	1.374695	0.031586	0.016661	0.136039	0.2499
NASA alloy 2	52.60618	11.57342	19.60531	6.289492	3.77153	0.932716	1.586344	0.124744	1.637093	1.420634	0.031664	0.016164	0.139158	0.265546
NASA alloy 3	51.82529	11.64886	20.23955	6.452008	3.762253	0.930422	1.595712	0.117711	1.626809	1.348569	0.029612	0.015049	0.133263	0.274889
NASA alloy 4	52.35668	12.74421	19.31623	5.973308	3.567281	0.857699	1.450271	0.140982	1.586217	1.385089	0.045975	0.010729	0.166259	0.399071
NASA alloy 5	51.52865	14.14501	18.88725	5.95665	3.582297	0.855307	1.423114	0.1272	1.581794	1.348727	0.039297	0.010699	0.165795	0.348214
NASA alloy 6	50.91574	12.45521	19.91644	6.462199	3.401442	0.889319	2.15549	0.142955	1.583087	1.454043	0.039958	0.010879	0.168585	0.404656
LSHR	48.21	14.5	20.67	7.52	4.24	0.9365	0.51	0	1.63	1.36	0	0	0.161	0.241
ME3	50.9	14.5	17.8	7.48	4.22	0.86	0.86	0	2.28	0.6	0	0	0.16	0.24

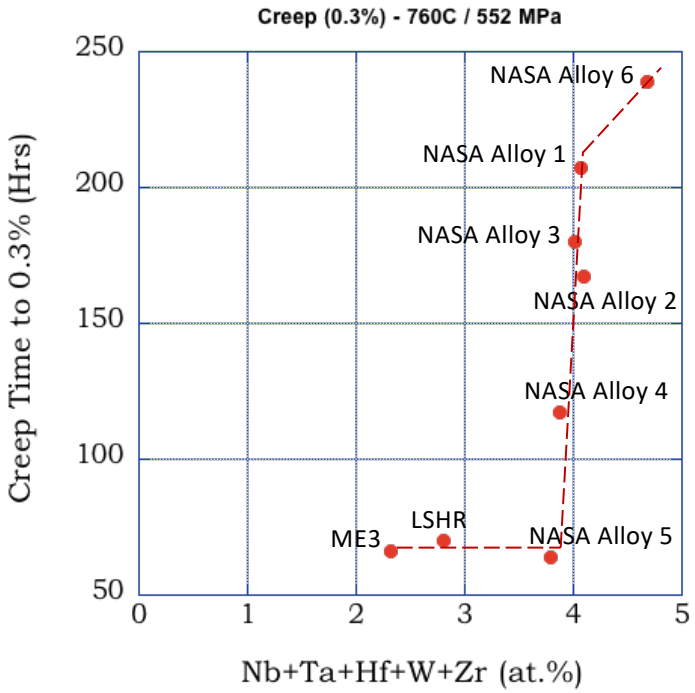
Distribution of elements at SISF in Ni_3Al-based γ'

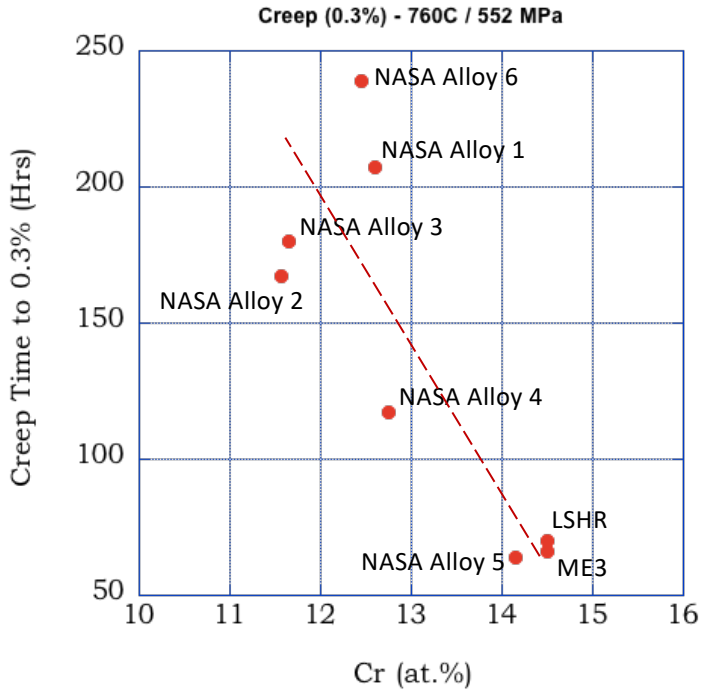


Atomic resolution characterization of a SISF in NASA Alloy 1

T. M. Smith *et al., Communications Materials,* 2 (2021) 1–9.

Experimental puzzle





Conclusions

- High temperature creep deformation in Ni-based superalloys was studied employing atomistic modeling.
- Our results indicate that relatively small addition of Nb can significantly slow down creep deformation of Ni-superalloys.
- Depending on the site preference of Cr in Ni_3Al γ' phase, two drastically different deformation behaviors can be expected.
- Cr on Al sites promotes twin growth via the Kolbe mechanism degrading the high temperature creep properties.
- Cr on Ni sites, on the other hand, suppresses twin growth and slows down the high temperature deformation creep.
- Our results explain the experimentally observed puzzling effects of elemental composition of the alloy on creep resistance.
- Cr site preference in γ' phase of Ni based superalloys can possibly be manipulated by tuning the alloy composition, thus, providing opportunity to design the next generation of Ni superalloys with improved creep resistance.