Twin nucleation and growth mechanism in Ni-based superalloys

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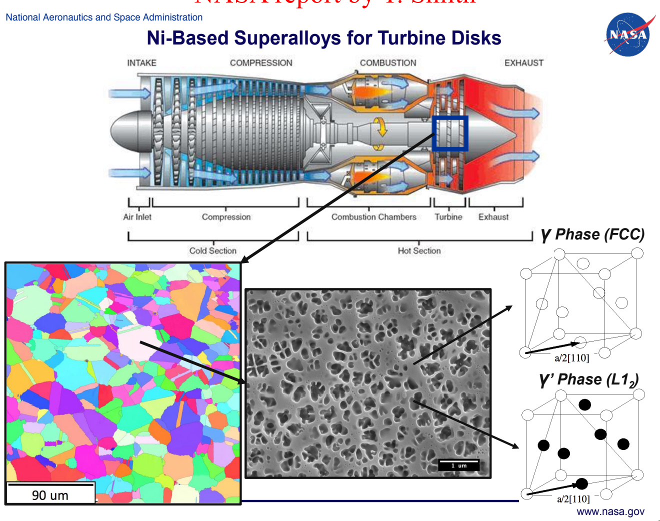
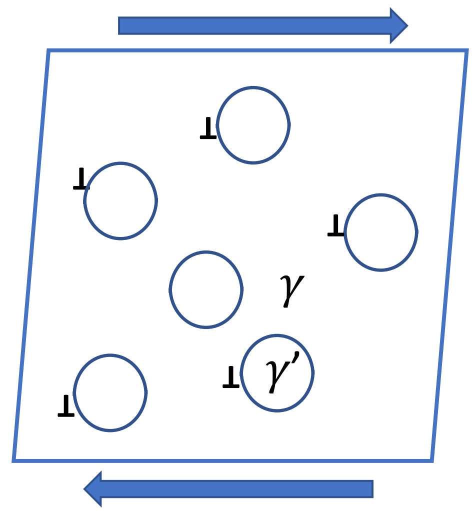
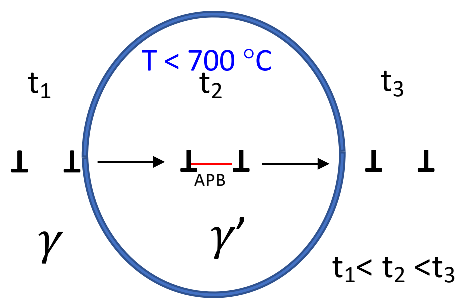
Deformation mechanisms in Ni-based superalloys

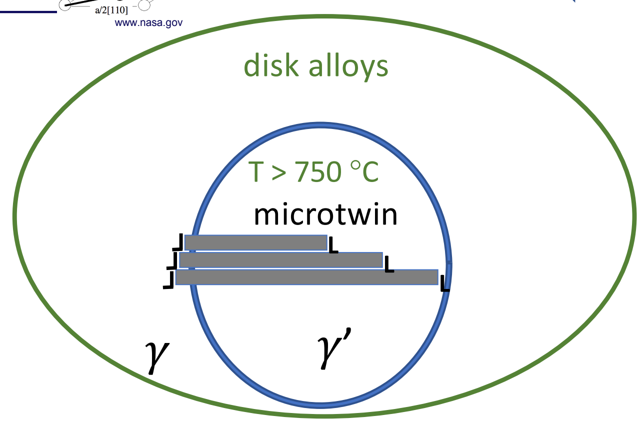
NASA report by T. Smith



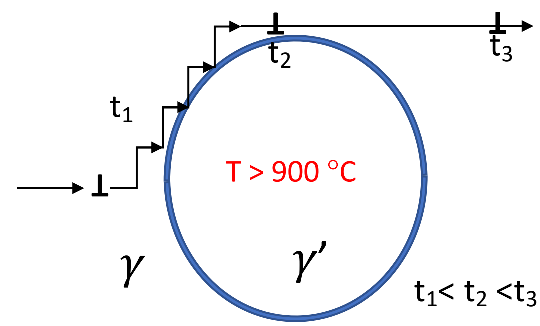


disk alloys





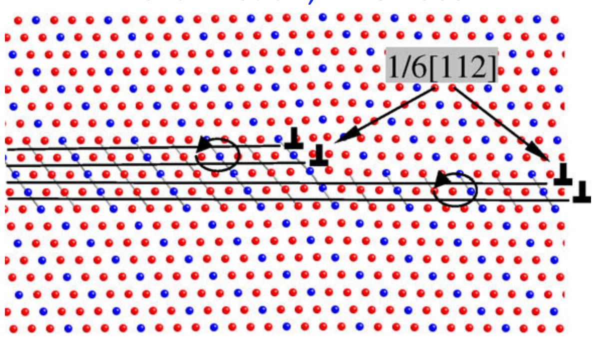
blade alloys



Micro-twinning in Ni-based superalloys

- Micro-twinning is a dominant 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

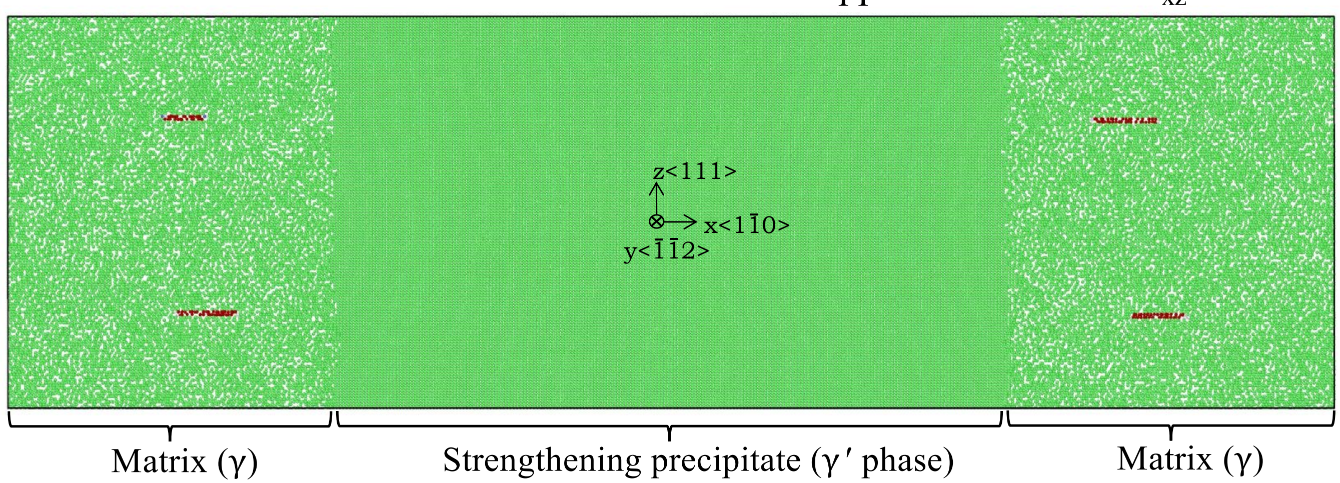


- We propose a qualitatively different mechanism for nucleation and growth of twins.
- The proposed mechanism is demonstrated via molecular dynamics simulations.

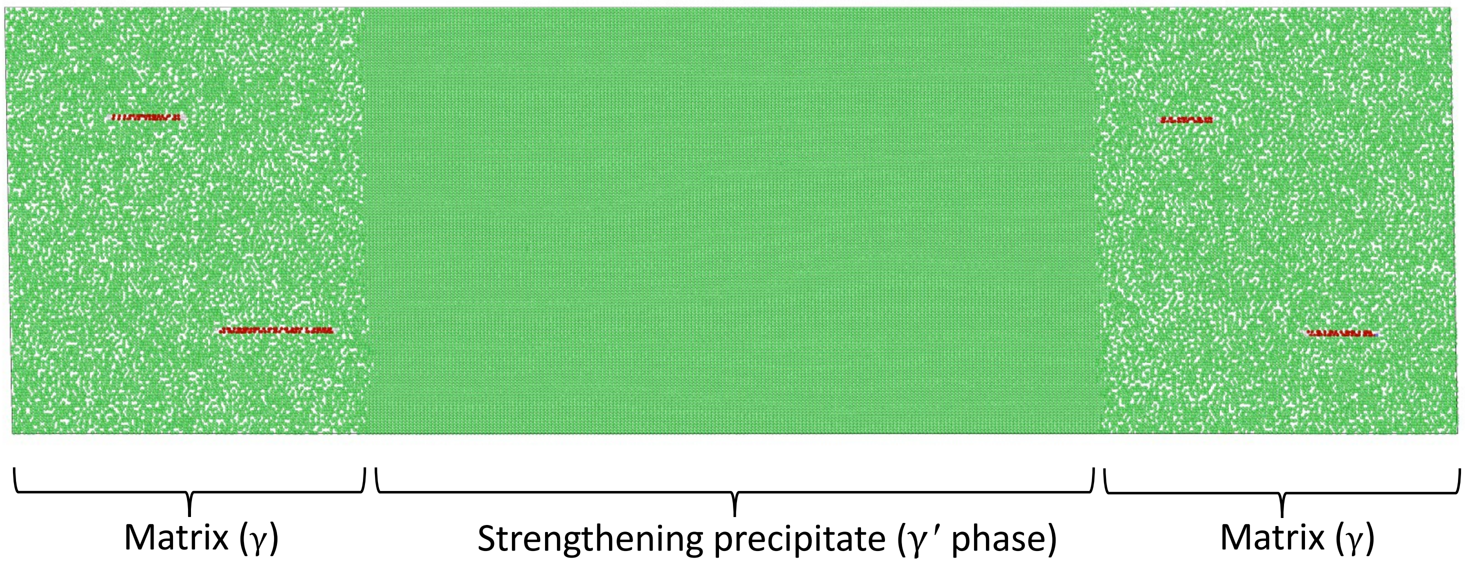
Micro-twinning in Ni-based superalloys

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: ~$100 \times 2.5 \times 29$ nm^3 (~700,000 atoms).
- PBCs in all directions.
- The system was relaxed at T = 1000K, 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 σ_{xz} shear stress was applied.
- The MD deformation simulations were carried out under applied shear stress σ_{xz} = 800 MPa.



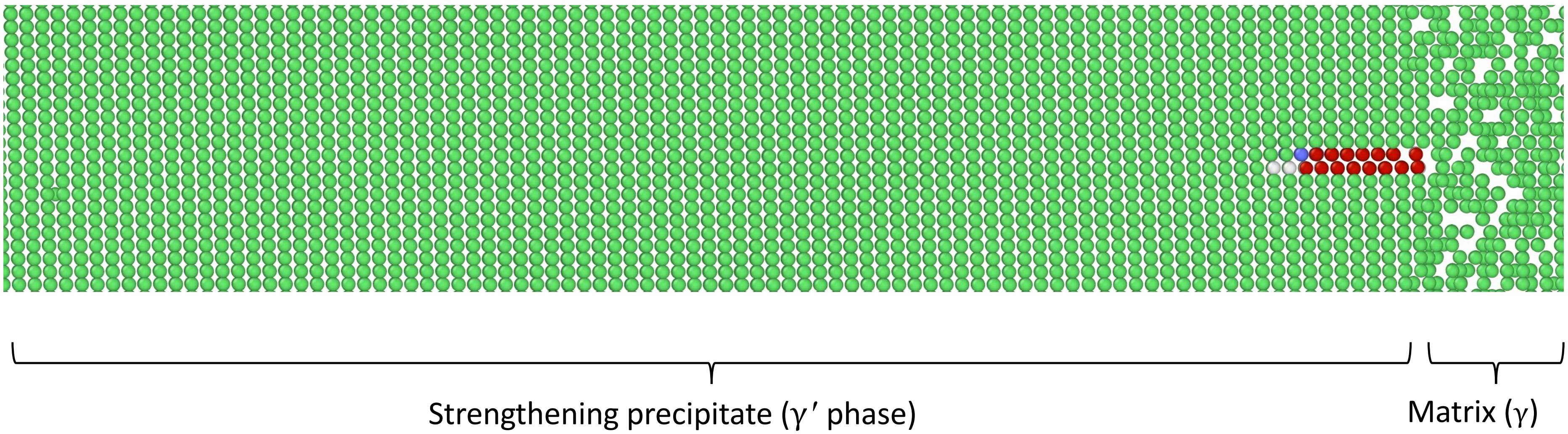
Discovered twin nucleation and growth mechanism



➢ The first step of twin nucleation and growth is formation of SISF inside precipitate.

Discovered twin nucleation and growth mechanism

SISF formation (discovered via MD simulation); colored according to lattice structure; Ni atoms are not shown



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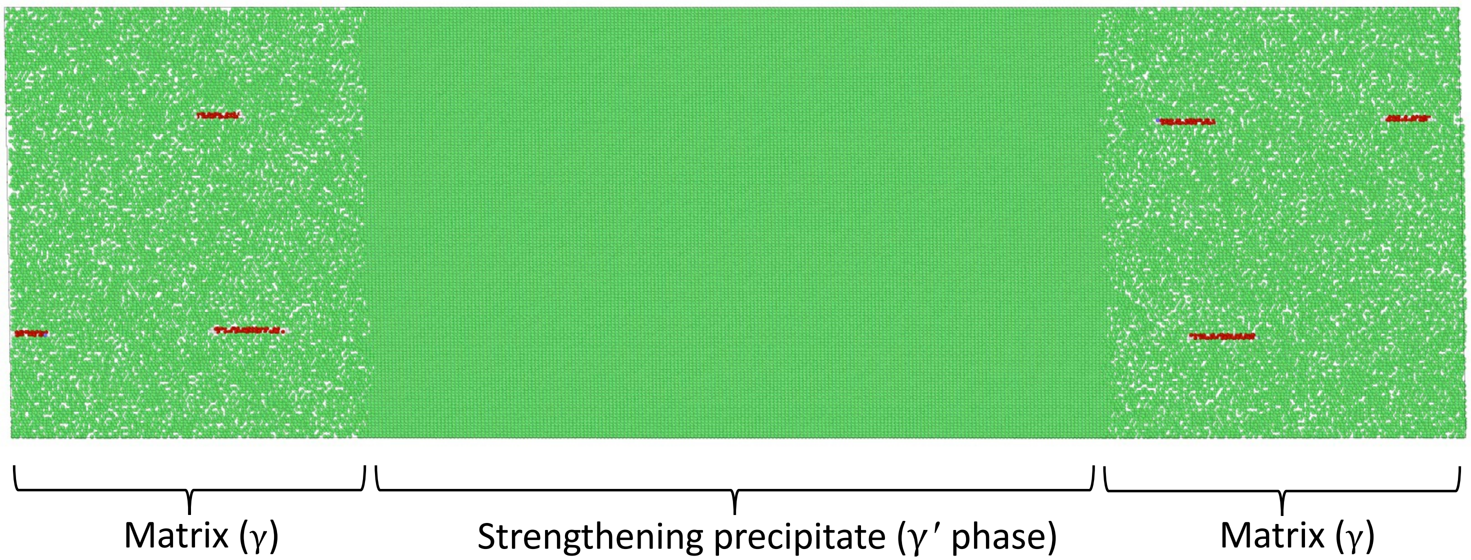
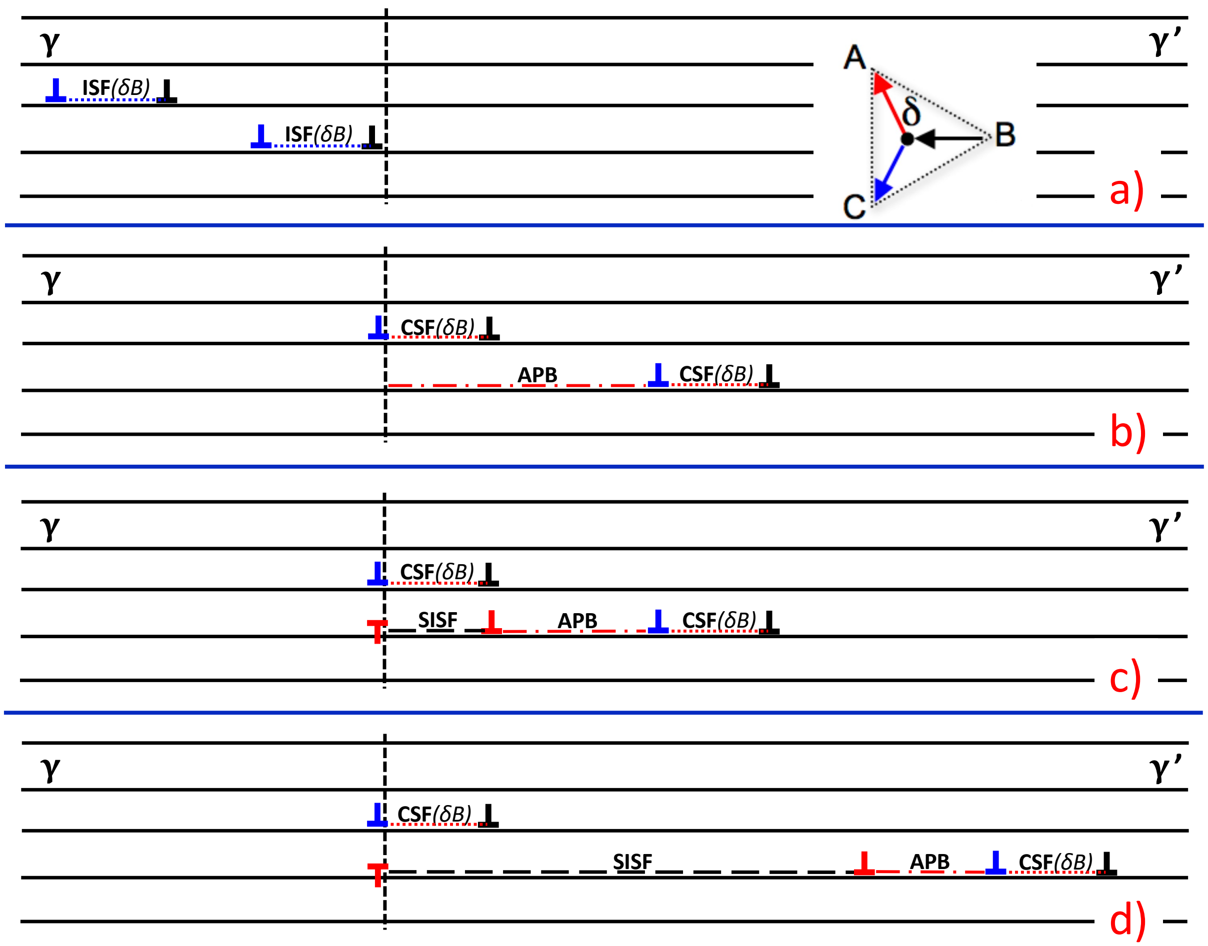
Discovered twin nucleation and growth mechanism



- The second step of twin nucleation and growth is formation of SESF inside precipitate.
- Recurring arrival of additional lattice dislocations from γ matrix will lead to growth of twin.

Discovered twin nucleation and growth mechanism



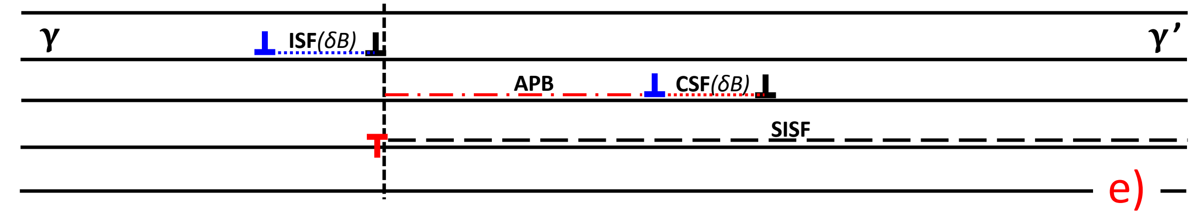
a) Arrival of the 1st BC dislocation to the interface

b) The 2nd BC dislocation, arriving to the interface (on the plane below) "pushes" the 1st one inside the precipitate (as a result, APB is produced).

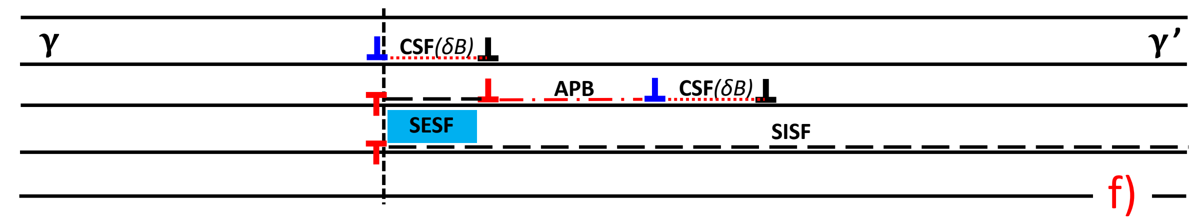
c) In addition, the arrival of the 2nd BC dislocation triggers nucleation and emission of A*δ* Shockley partial (at the interface, on the glide plane of the 1st BC dislocation). This converts APB left by the 1st BC into SISF.

d) The A*δ* Shockley quickly propagates towards the 1st BC dislocation, extending SISF into the precipitate.

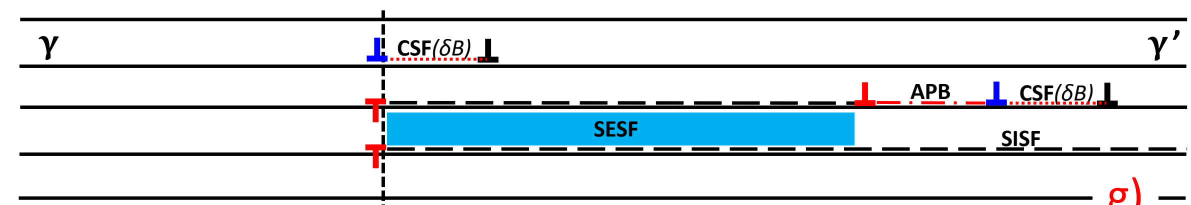
Discovered twin nucleation and growth mechanism



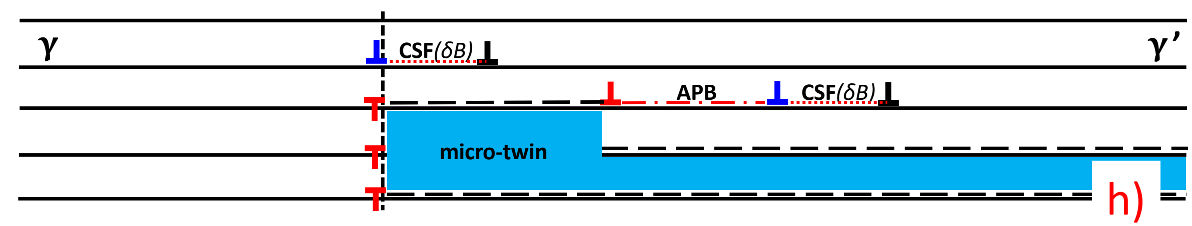
e) Following the same logic, arrival of another BC dislocation one plane above the configuration depicted in d) will trigger the repetition of the processes described in c)-d) on the corresponding planes.



f) In particular, the arrival of the 3rd BC dislocation will trigger nucleation of yet another Aδ Shockley leading to formation of SESF embryo.



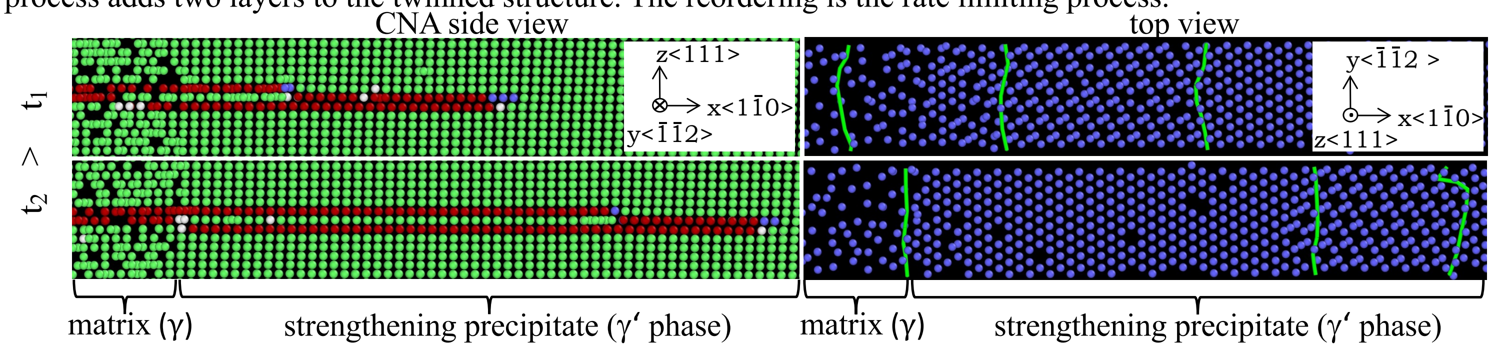
g) Propagation of this Aδ Shockley into precipitate will remove APB left by the 2nd BC dislocation and extend the SESF into precipitate.



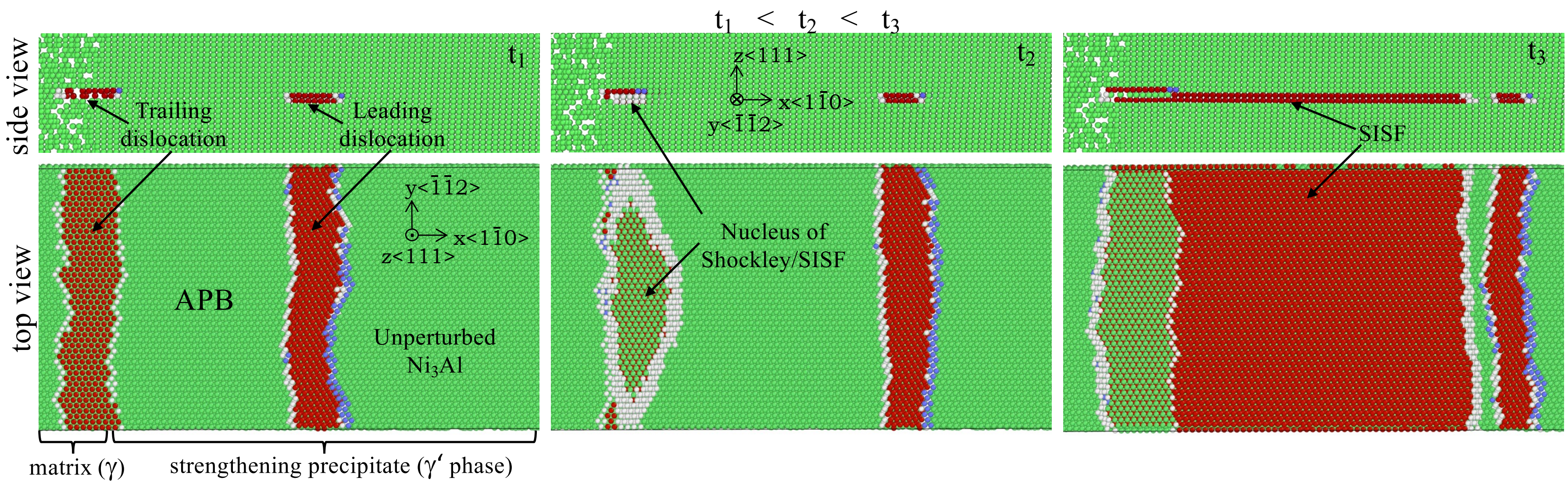
h) Recursive arrival of additional BC dislocations on the planes above the configuration depicted in g) will lead to formation and growth of the twin.

Comparison with the Kolbe mechanism

- In the Kolbe mechanism twin can grow only due to passage of two Shockley partials that create 2-layer CSF that can be reordered. The process adds two layers to the twinned structure. The reordering is the rate limiting process.

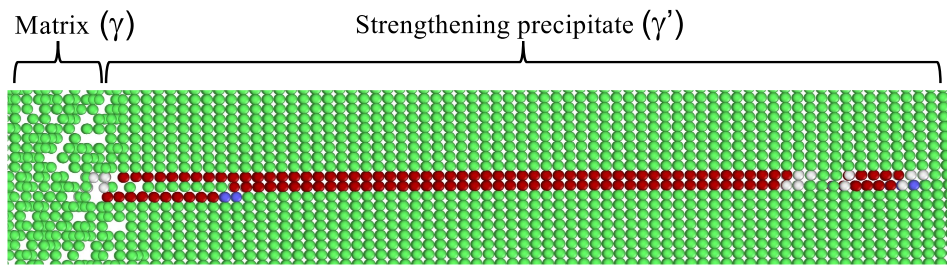


- In the proposed mechanism reordering is not involved. The rate limiting process is nucleation of Shockley partial. Single step adds one layer.

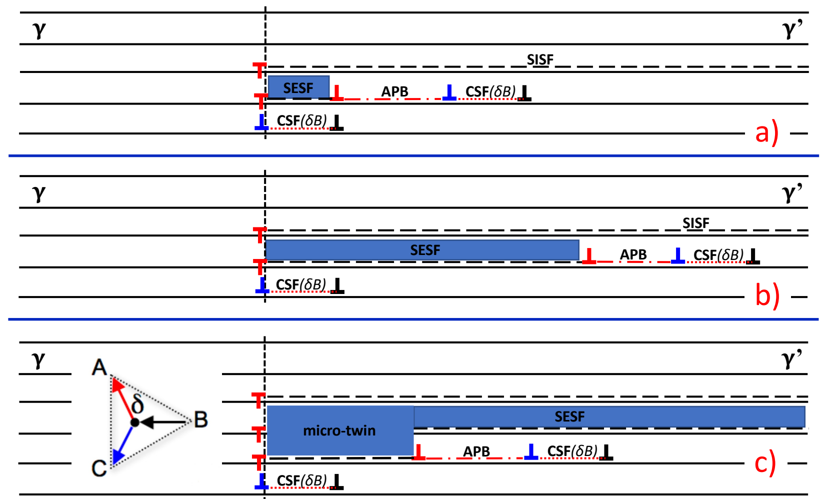


Conclusions

- We propose a new twin nucleation and growth mechanism in Ni-superalloys.
- It is qualitatively different from the Kolbe mechanism.
- The rate-limiting process in the Kolbe mechanism is thermally activated reordering (via vacancy diffusion).
- The rate-limiting process of the new mechanism is nucleation of the Shockley partial.
- Studying rate-limiting processes of both mechanisms will allow us to propose changes in alloy composition, that would make the material stronger.



The first step of new twin growth mechanism: formation of super intrinsic stacking fault (SISF)



Schematics of the discovered twin growth mechanism