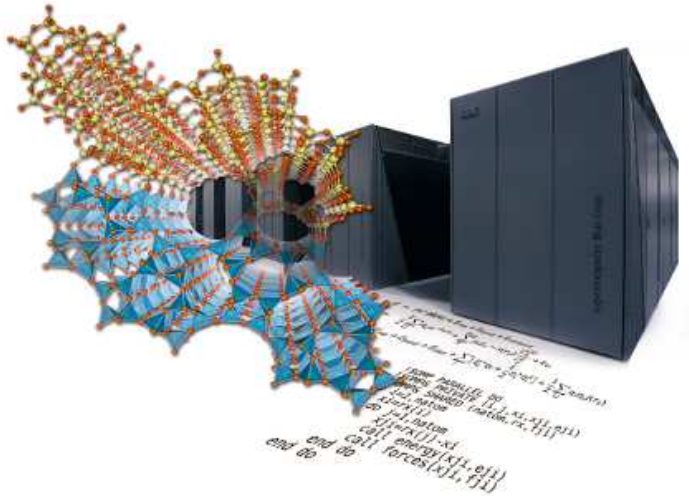
Study of grain boundary deformation mechanisms in cemented carbides using a model potential for the W-C-Co system



Force Fields 2014

Gren M., Petisme M., and Wahnström G.

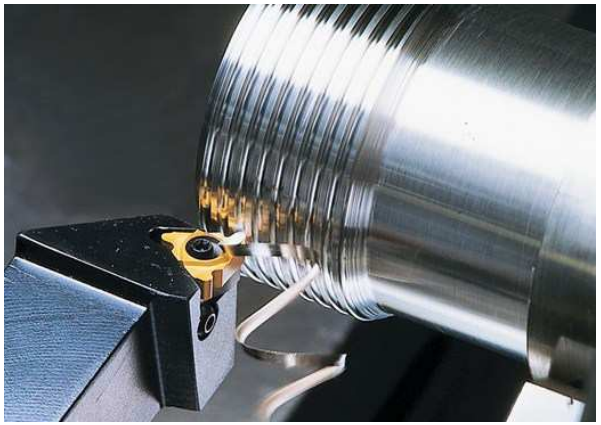
Department of Applied Physics,
Chalmers University of Technology

Workshop on Force Fields: From Atoms to Materials, Monday 3 November, 2014

Outline

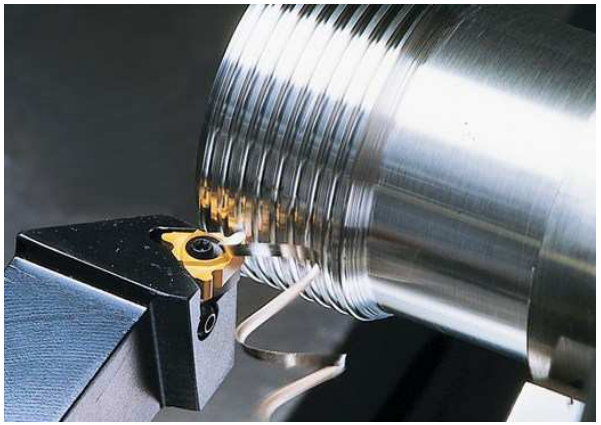
Cemented carbide

- Pure WC hard and brittle



Cemented carbide

- Pure WC hard and brittle
- Adding ductile metal binder
  $\Rightarrow$ unique combination of hardness and toughness



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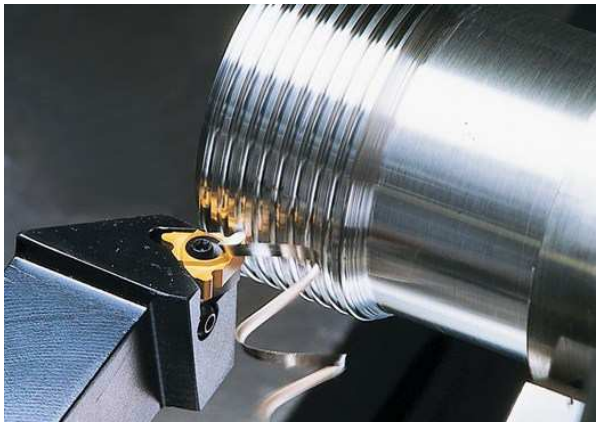

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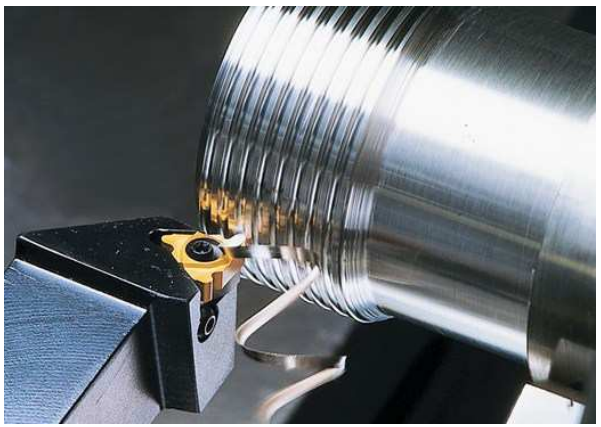

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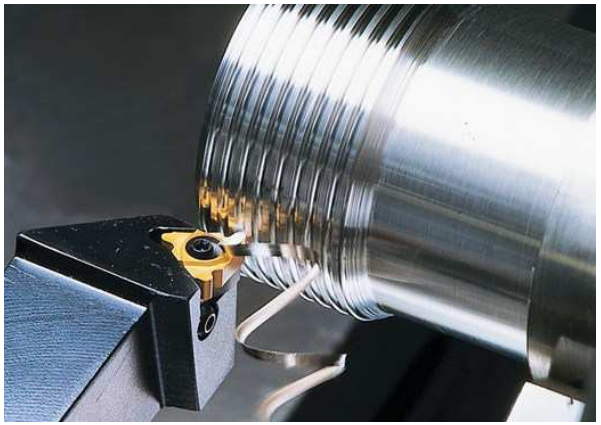
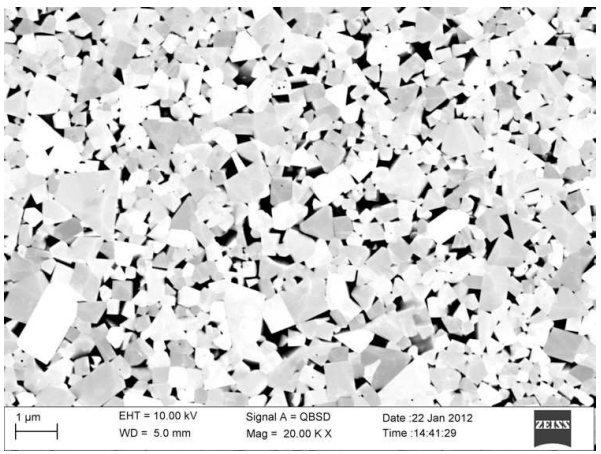
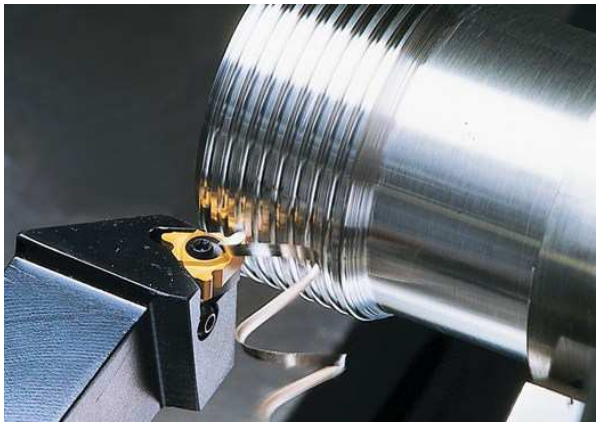


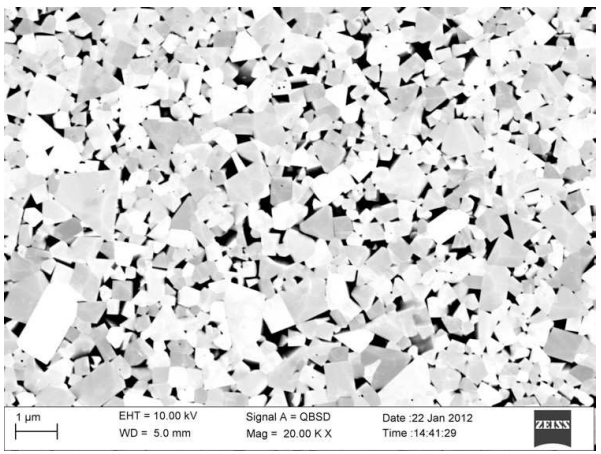


Typical microstructure, $\sim$6 wt-% Co (WC: light, Co: dark)

Cemented carbide

Plastic deformation of bulk material often limits tool life at high T





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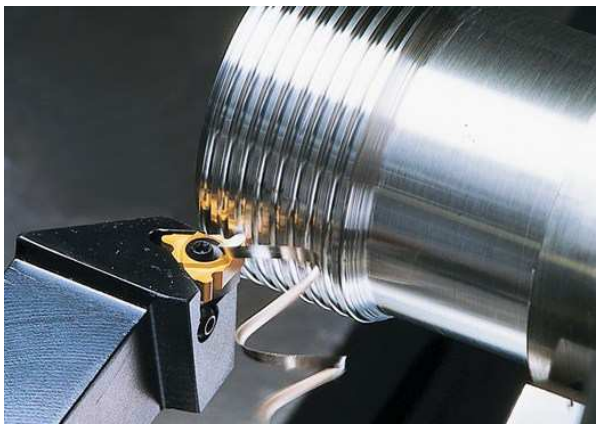

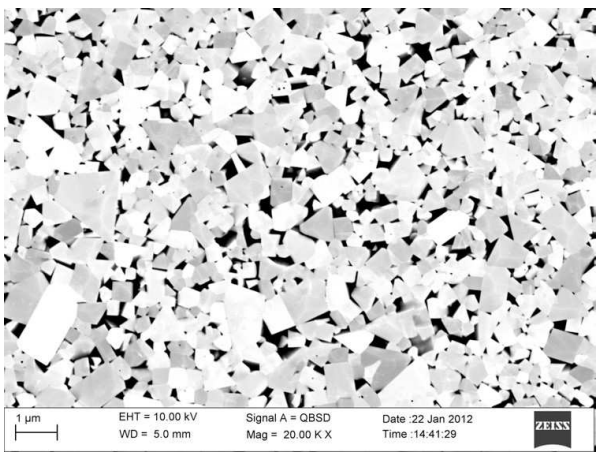

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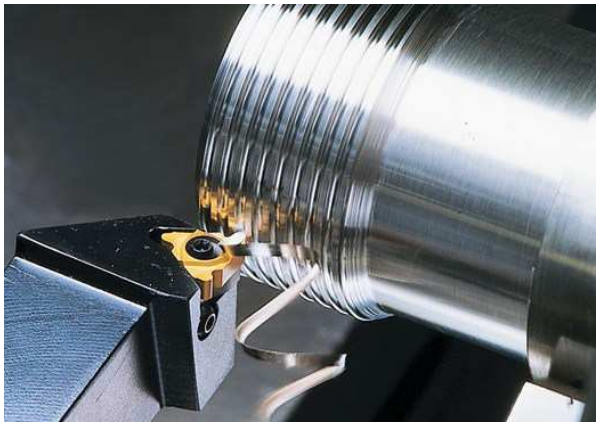
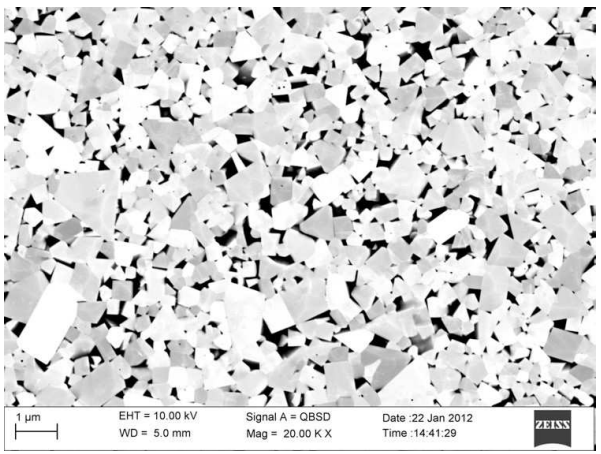
Cemented carbide

Plastic deformation of bulk material often limits tool life at high T

Suggested mechanism:

- Rigid WC skeleton broken up and WC/WC grain boundaries infiltrated by Co
- Deformation occurs by grain boundary sliding (gbs) facilitated by Co infiltration





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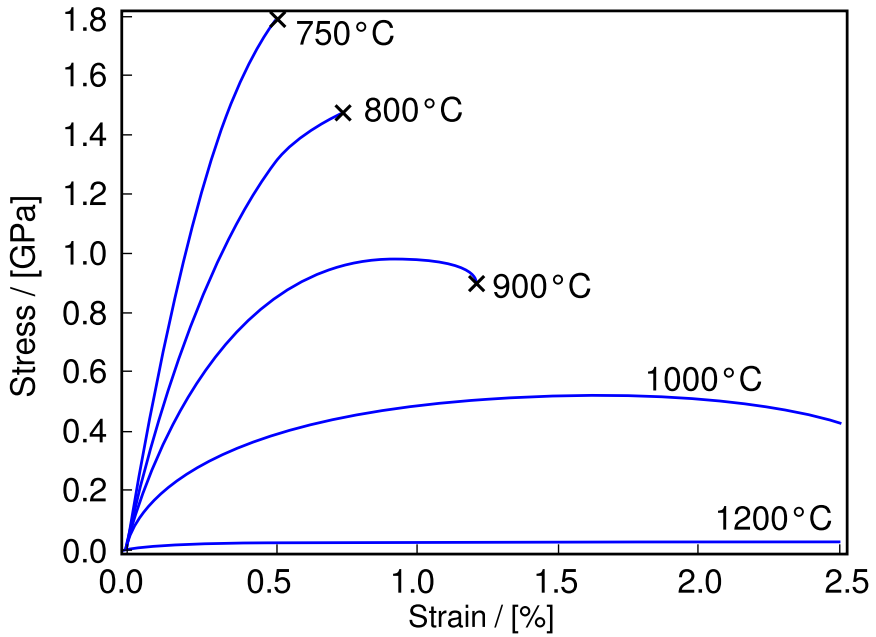
Experimental support for gbs (3-point bending and SEM)*

WC–Co undergoes gradual ductile–brittle transformation



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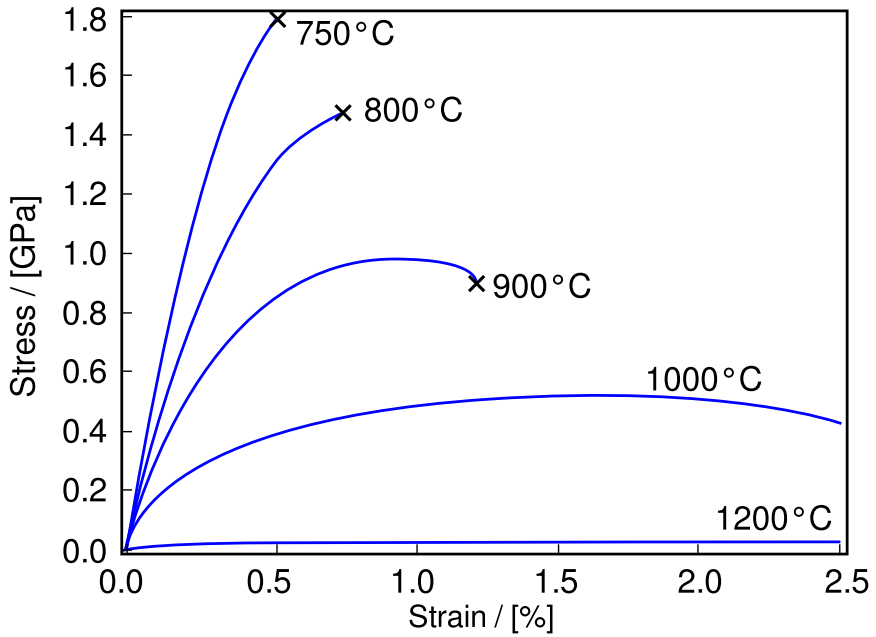

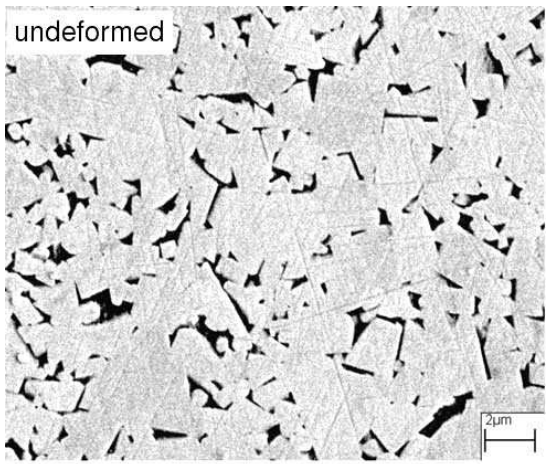

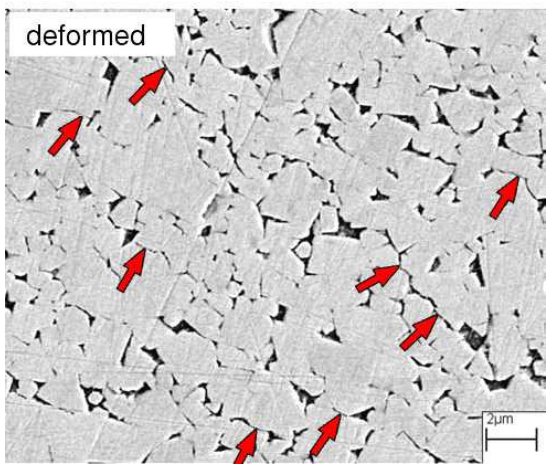

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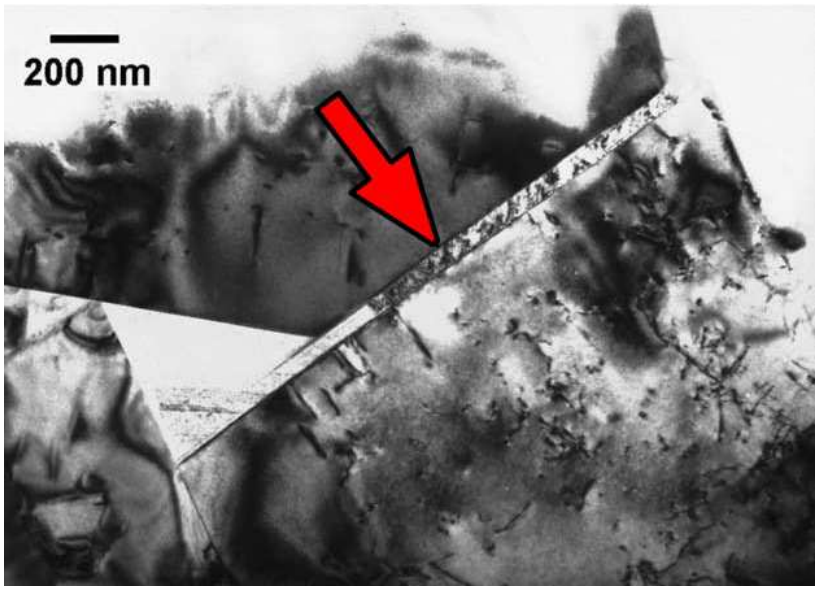
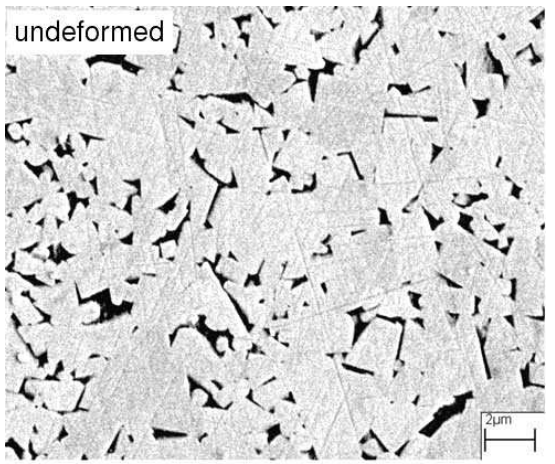
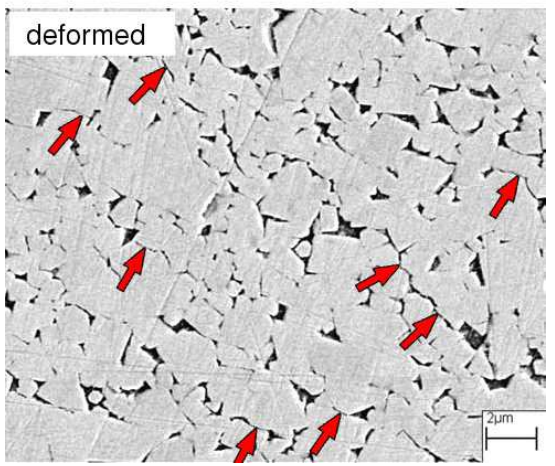
Experimental support for gbs (3-point bending and SEM)*

Co lamellae seen in deformed sample







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We have studied gbs and Co infiltration using molecular dynamics with an interatomic potential for the W-C-Co system.

Interatomic potentials

- We use an *analytical bond order potential* (ABOP) of Tersoff–Brenner type with 9 parameters per interaction type:

$$E_{\text{abop}} = \sum_{i>j} \{ V_{\text{repulsive}}(r_{ij}) - b_{ij} V_{\text{attractive}}(r_{ij}) \}$$

  where b_{ij} includes environmental dependence, including angularity.
- For the W–C system we use the parameters of Juslin *et al.*[*]
- We have developed Co parameters using standard ABOP approach[**]
- T_m for Co well described, 1750±50 K (1768 K exp.)

[*] Juslin N. *et al.*, J. Appl. Phys. **98**, 12, 123520 (2005)
[**] Albe K. *et al.*, Phys. Rev. B **65**, 195124, (2002)

Interatomic potentials

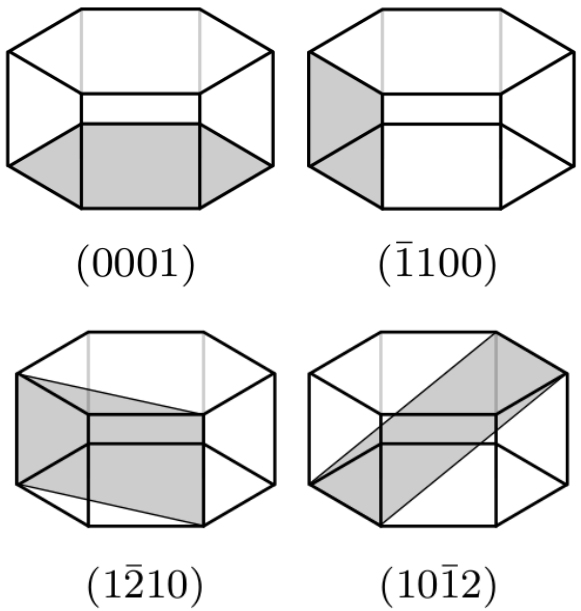
- Co–C and Co–W parameters developed using mainly force-matching[†] to first-principles DFT data[‡]
- C and W dissolved in Co
- WC/Co interfaces
- Segregation energies for Co in WC grain boundaries

[†] F. Ercolessi and J. B. Adams, Europhys. Lett. **26**, 583 (1994)
[‡] M.V.G. Petisme, S.A.E. Johansson, G. Wahnström, Proc. Int. Plansee Sem. 2 (2013).

Grain boundary sliding

Choosing model grain boundaries

- Most common planes in WC/WC grain boundaries are basal and prismatic*
- We also utilize DFT to determine interface segregation.** In this case we use the coherent approximation and need to use grain boundaries with a low Σ.



*Kim, C.–S. and Rohrer, G. S., Interface Sci. **12**, 19 (2004)

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Choosing model grain boundaries

- Most common planes in WC/WC grain boundaries are basal and prismatic*
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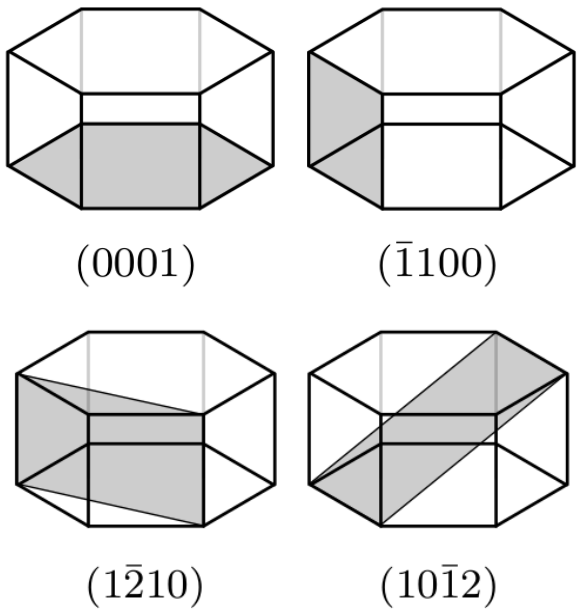
- $\Rightarrow$ We choose:
  - $\Sigma 2$ tilt grain boundary with one (0001) and one $(1\bar{2}10)$ plane
  - $\Sigma 4$ tilt grain boundary with one $(\bar{1}100)$ and one $(10\bar{1}2)$ plane



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Misfit in grain boundary

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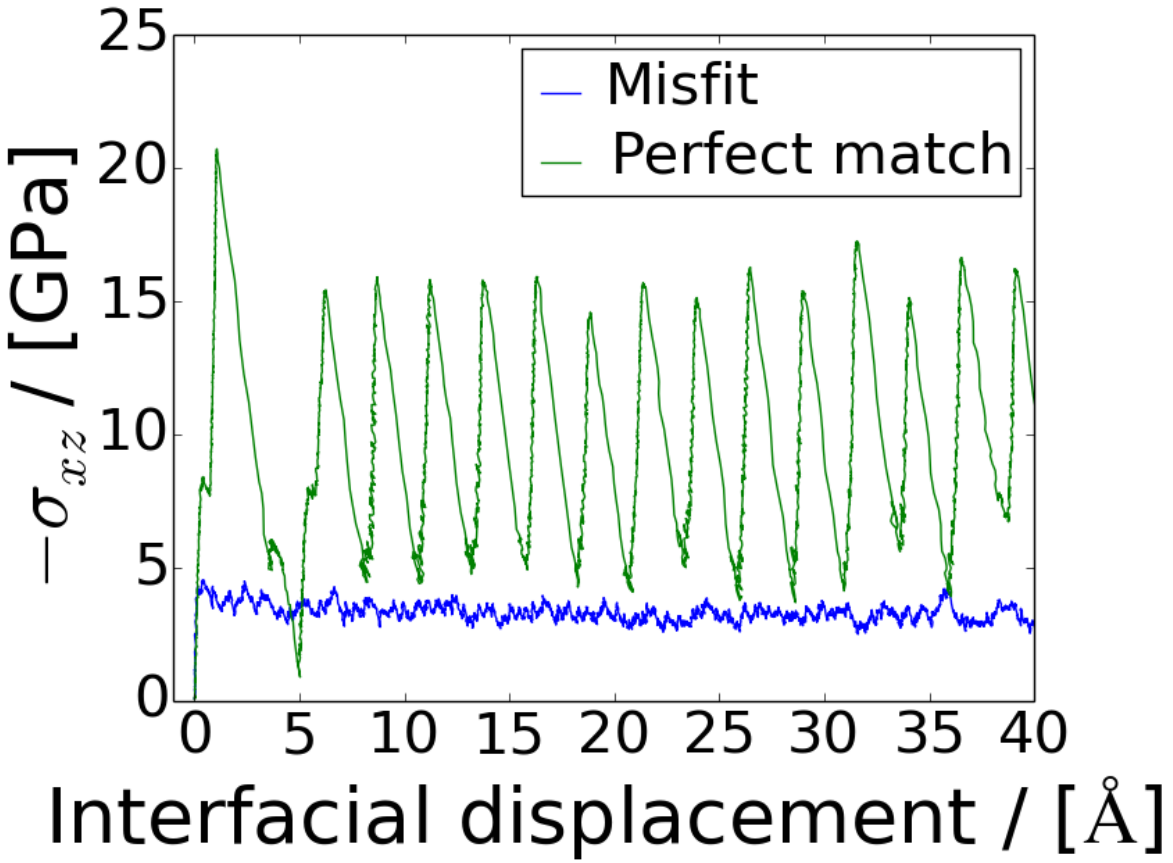

Clean $\Sigma 2$ grain boundary at 300 K

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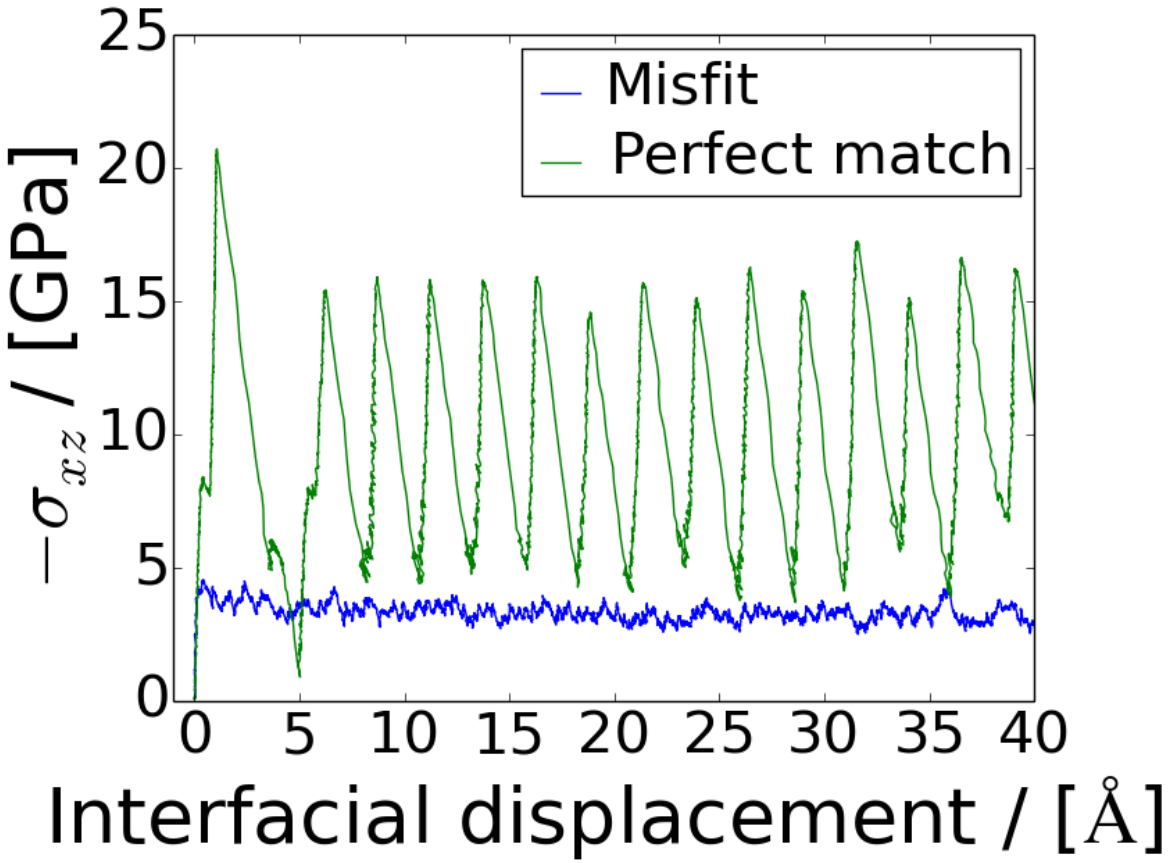
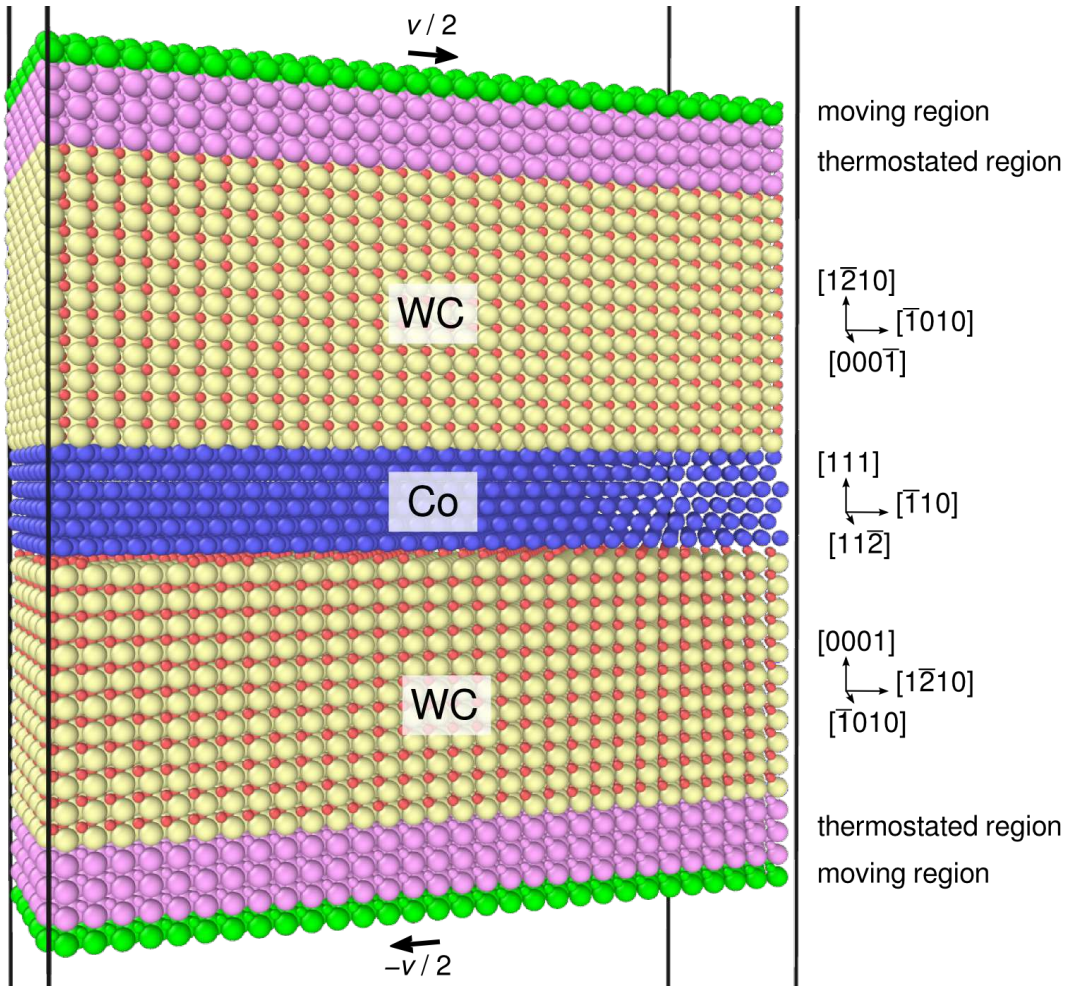


Clean $\Sigma 2$ grain boundary at 300 K

$\Rightarrow$ We look at sliding in direction with misfit

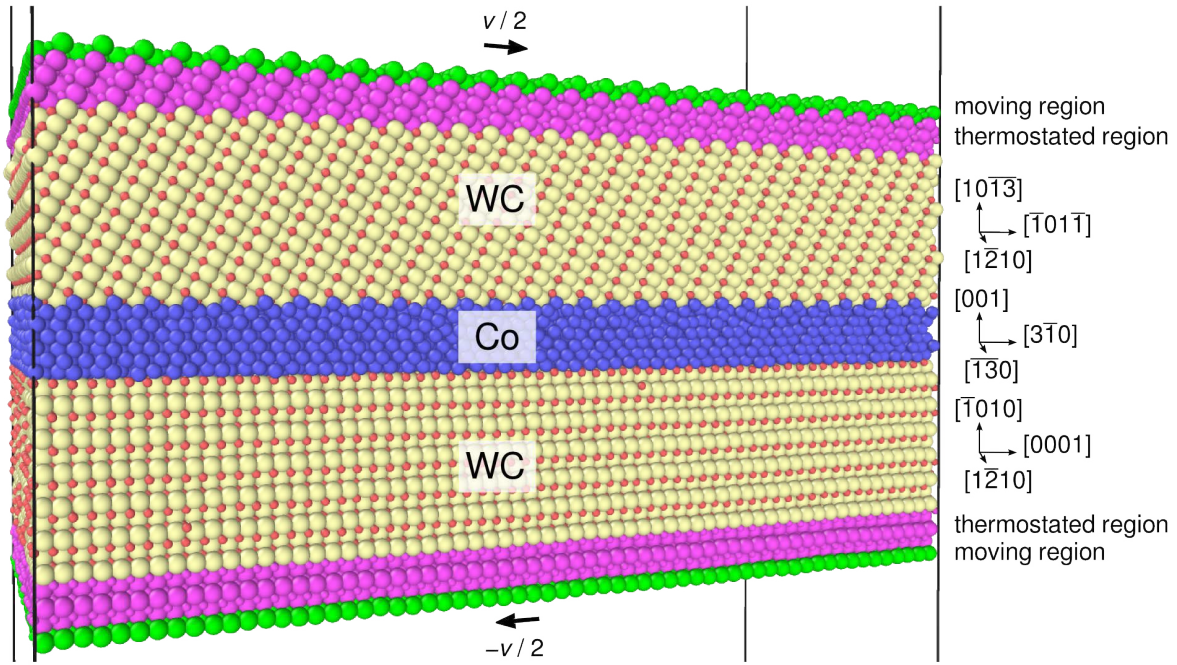
Model system 1 – Σ2 with misfit

- Σ2 90° $[\bar{1}010]$ tilt grain boundary
- Sliding at 0.1 Å/ps
- Thermostated layers
- Strain due to commensurate cell $\sim 0.4\,\%$
- $\sim$ 25,000 atoms



Model system 2 – Σ4 with misfit

- Simulation done as for Σ2.
- Σ4 60° $[1\bar{2}10]$ tilt grain boundary
- Strain due to commensurate cell ∼ 0.6 %
- ∼ 100,000 atoms

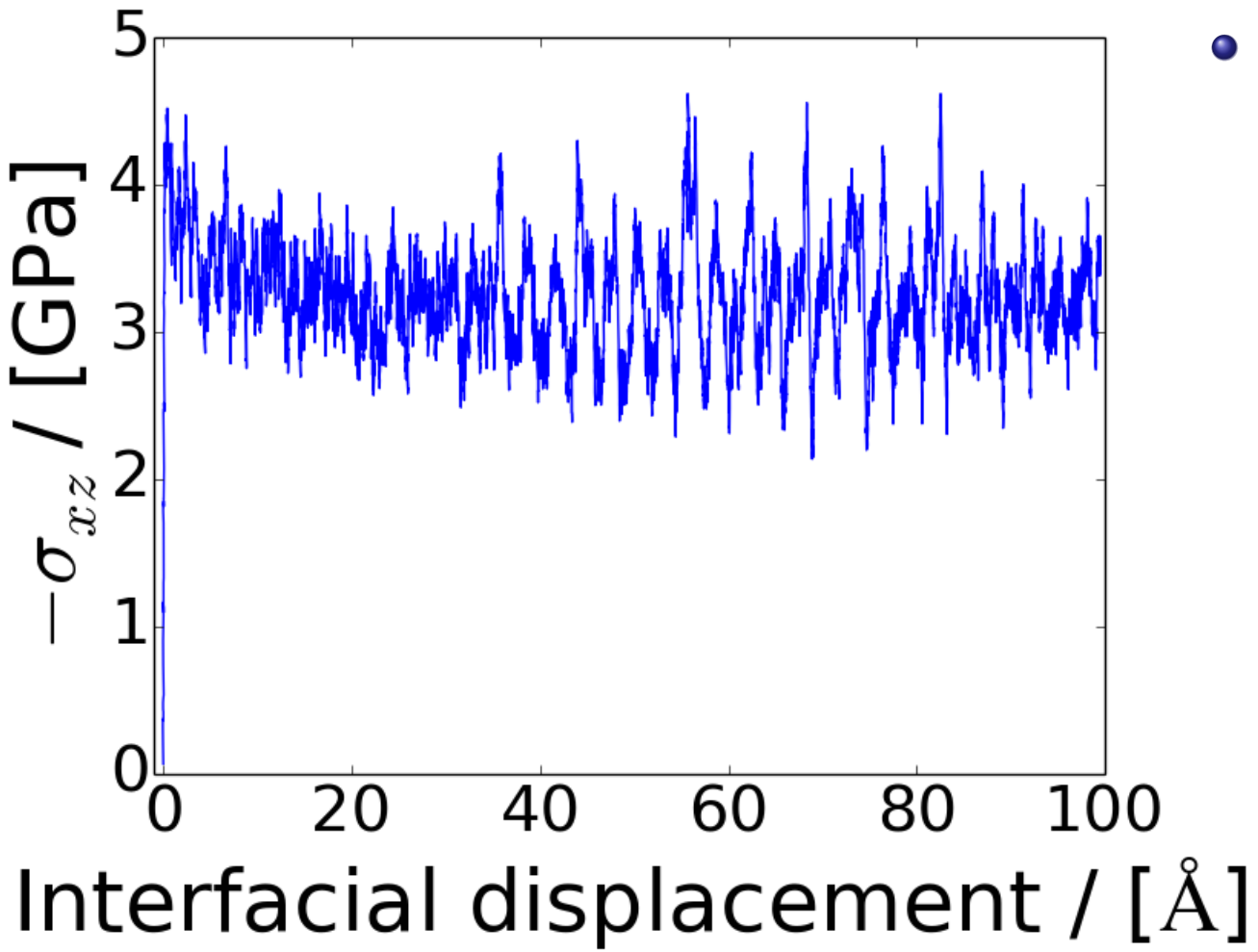


Simulation methodology

- Molecular Dynamics (MD) as implemented in the LAMMPS code
- Constant sliding speed 0.1 Å/ps imposed away from interface
- Timestep 1 fs, simulation time 1 ns.
- Zero pressure normal to the interface
- Measure resulting shear stress using

$$\sigma_{ij} = \frac{1}{N}\sum_k \beta_{ij}^k \quad \text{where} \quad \beta_{ij}^k = -\frac{1}{V_k}\left\{ m v_i v_j + \frac{1}{2}\sum_{\ell \neq k} f_i^{k\ell} r_i^{k\ell} \right\}$$

Results, clean GB as an example



- Shear stress as function of interfacial displacement

Clean $\Sigma 2$ grain boundary at 300 K

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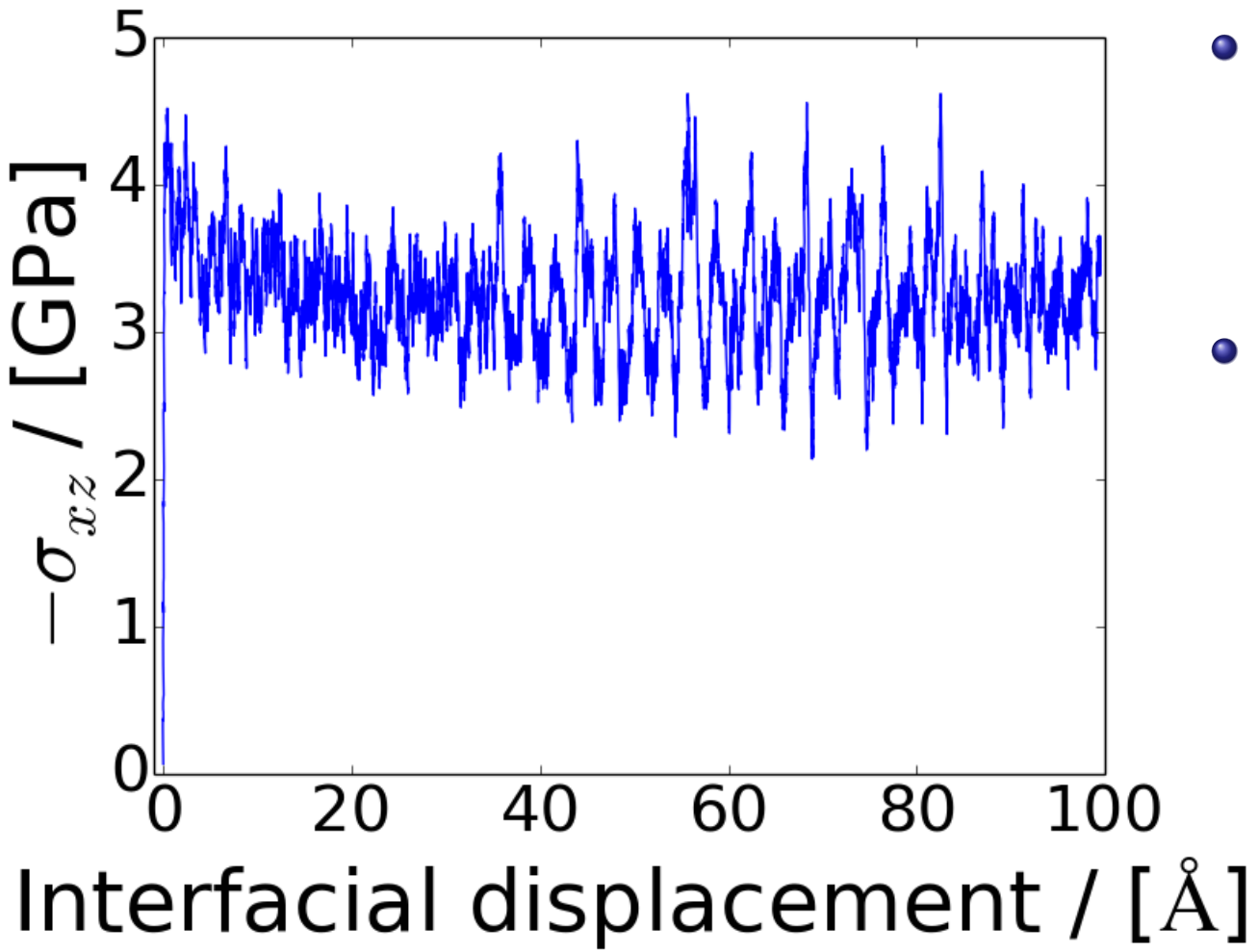

- Shear stress as function of interfacial displacement
- We use 6 simulations to calculate averages and error bars

Clean $\Sigma 2$ grain boundary at 300 K

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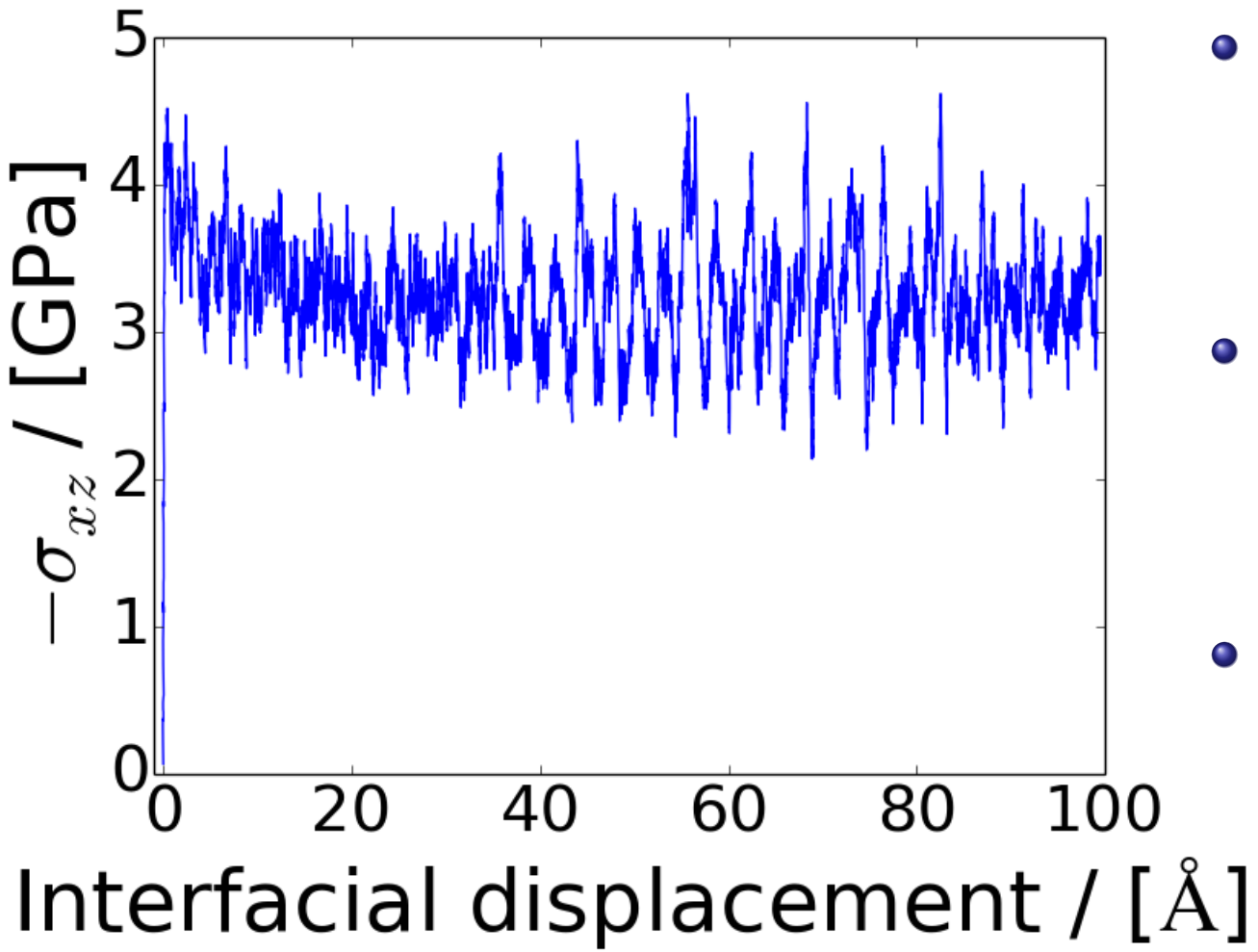
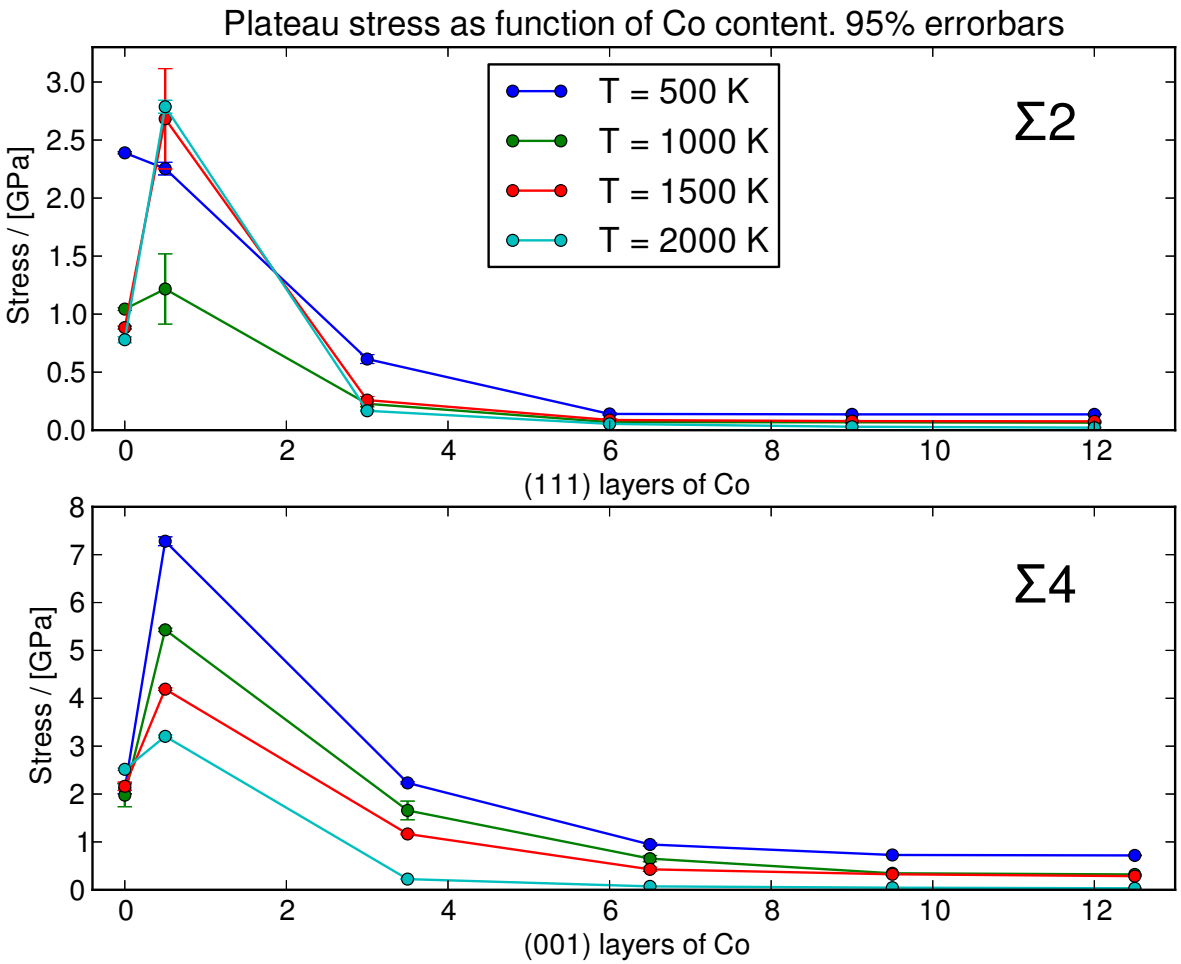


Clean $\Sigma 2$ grain boundary at 300 K

- Shear stress as function of interfacial displacement
- We use 6 simulations to calculate averages and error bars
- We take the plateau stress as the average of the last third of the simulation

Results as function of Co content and T



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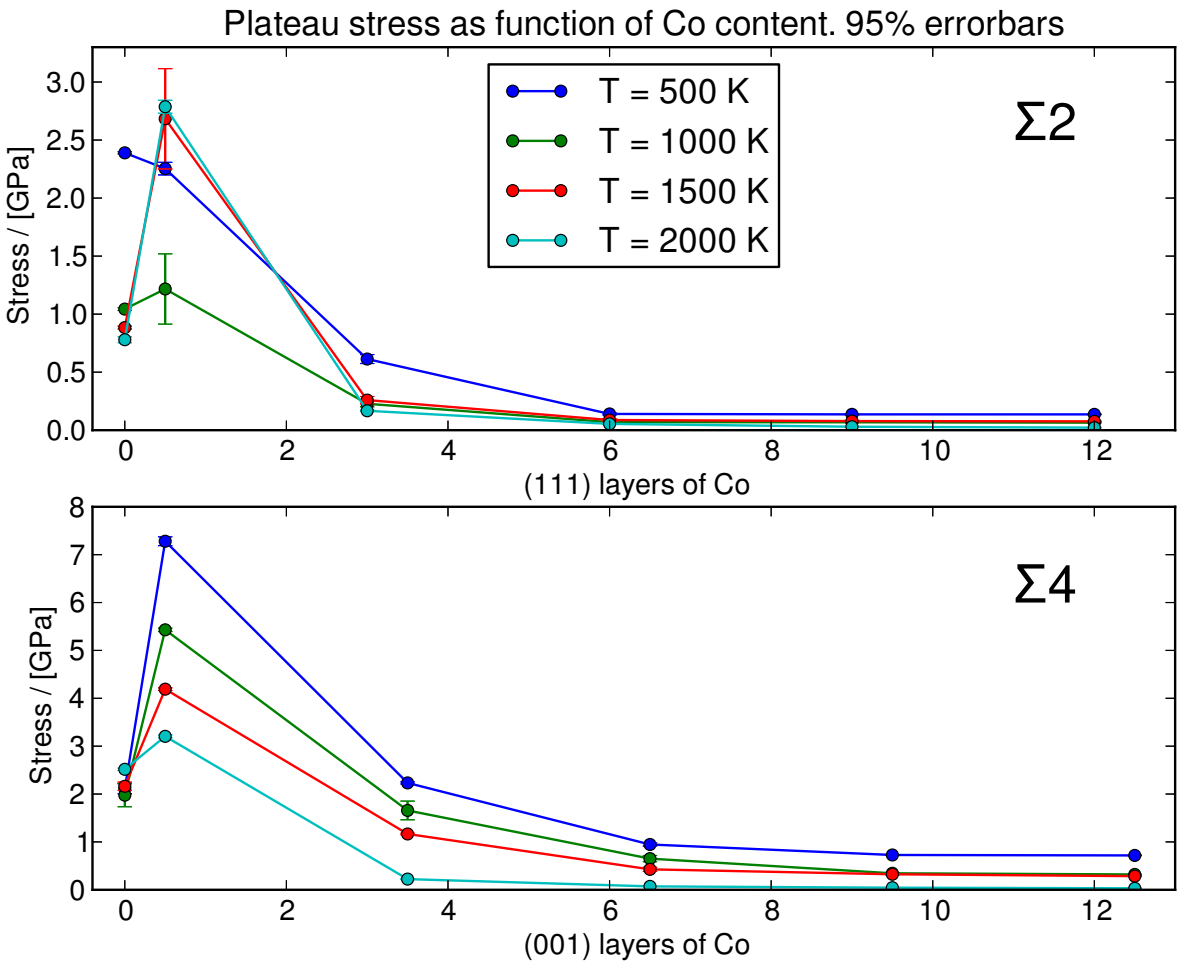

Observations

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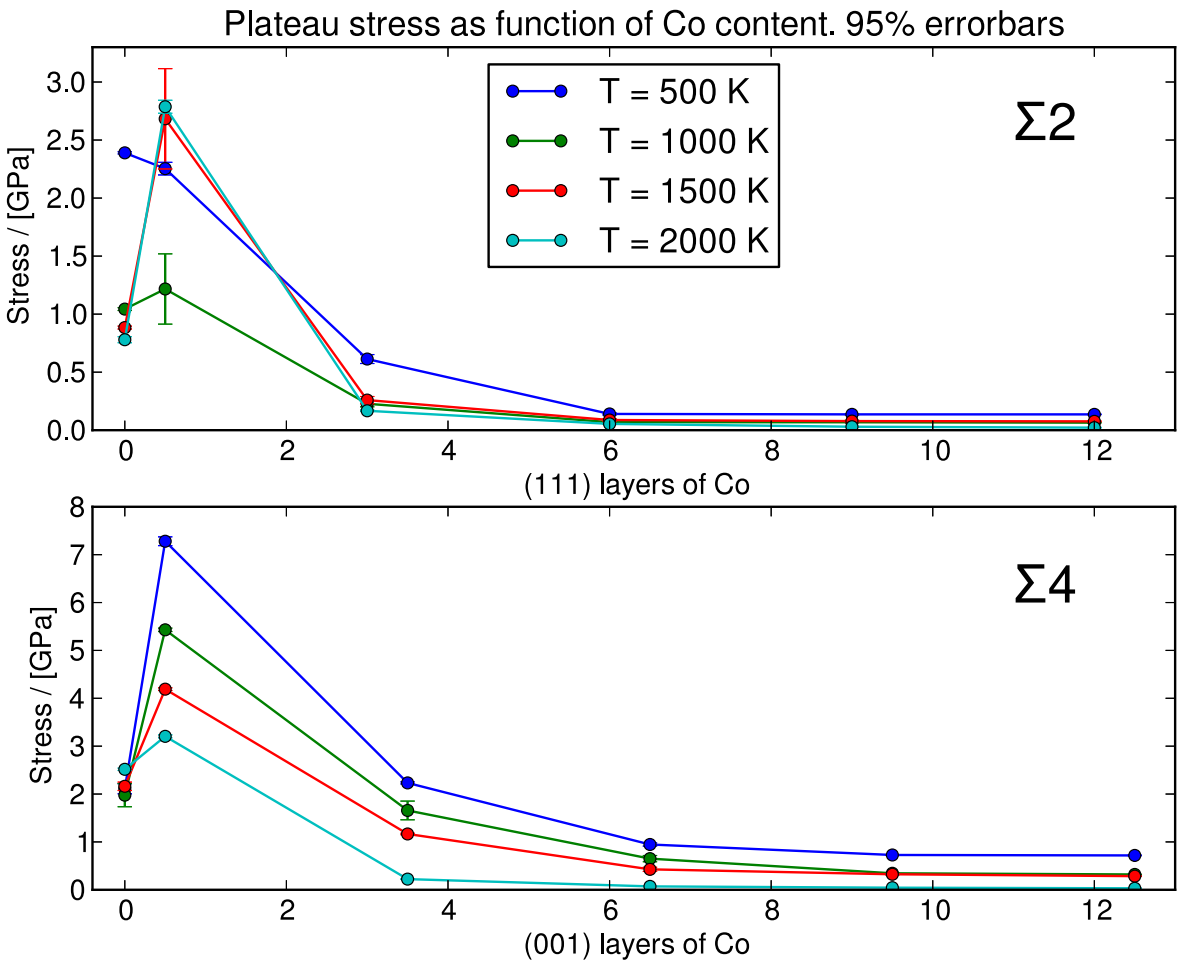
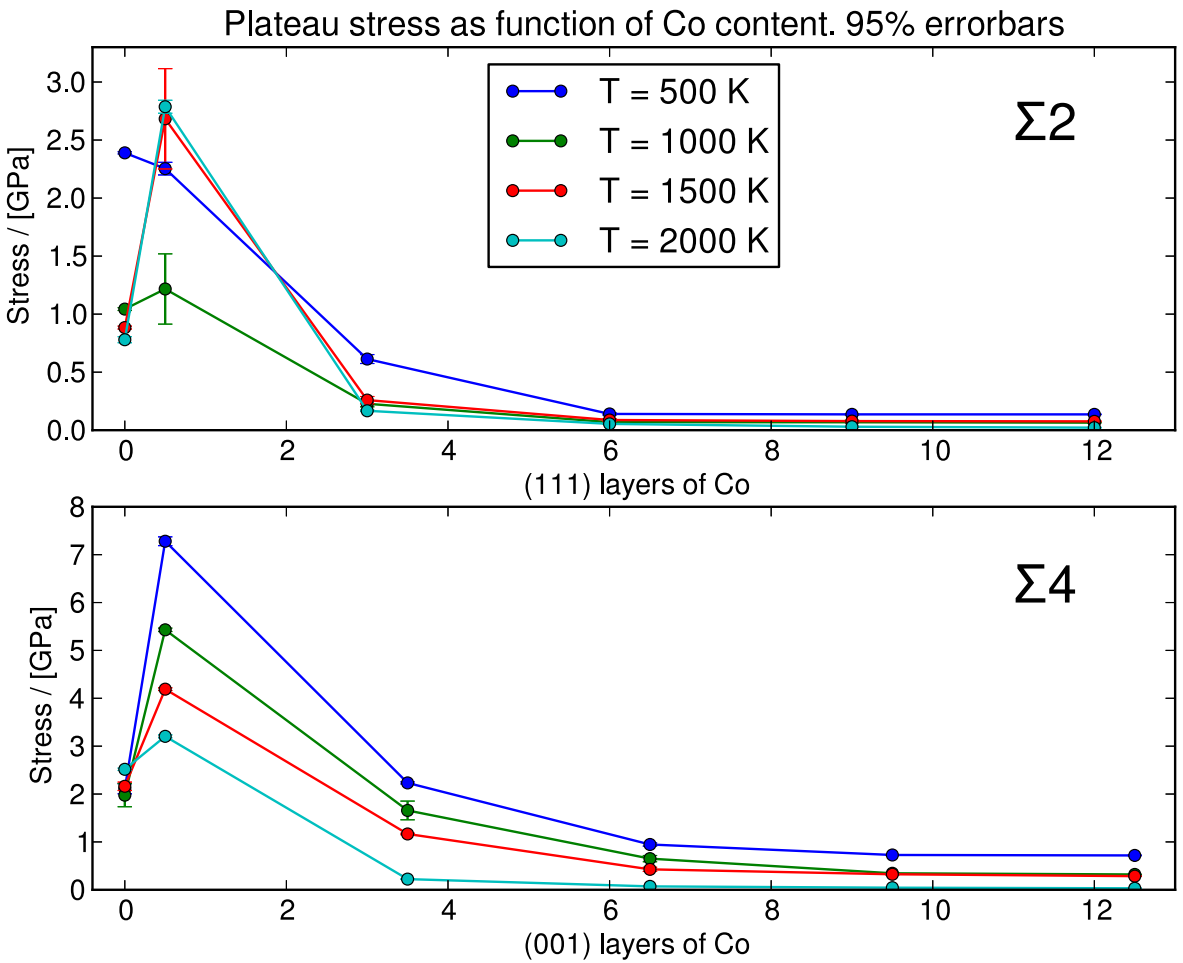


Observations

1. Co infiltration significantly facilitates gbs

Results as function of Co content and T



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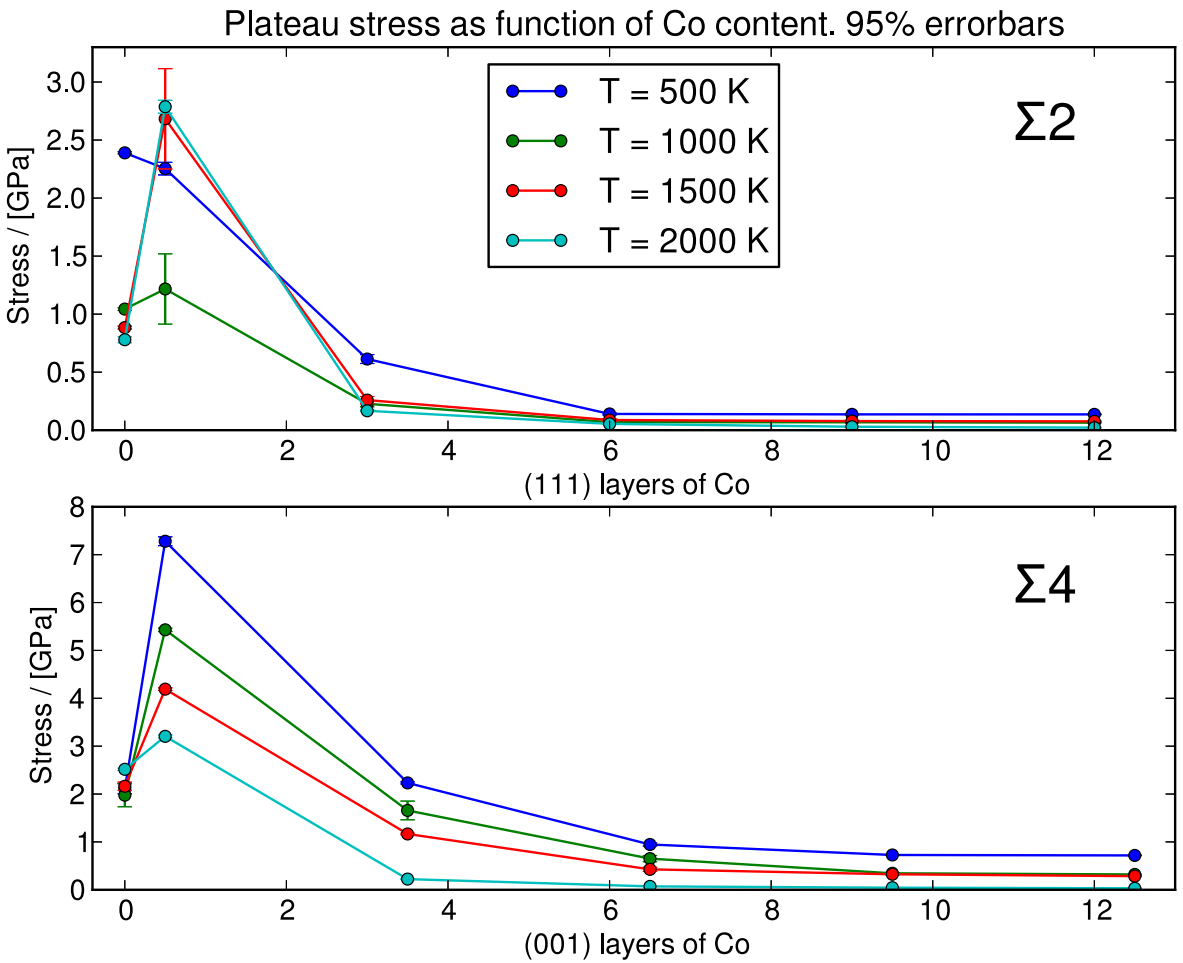
2. A few layers, ~ 1 nm, of Co are required to facilitate gbs

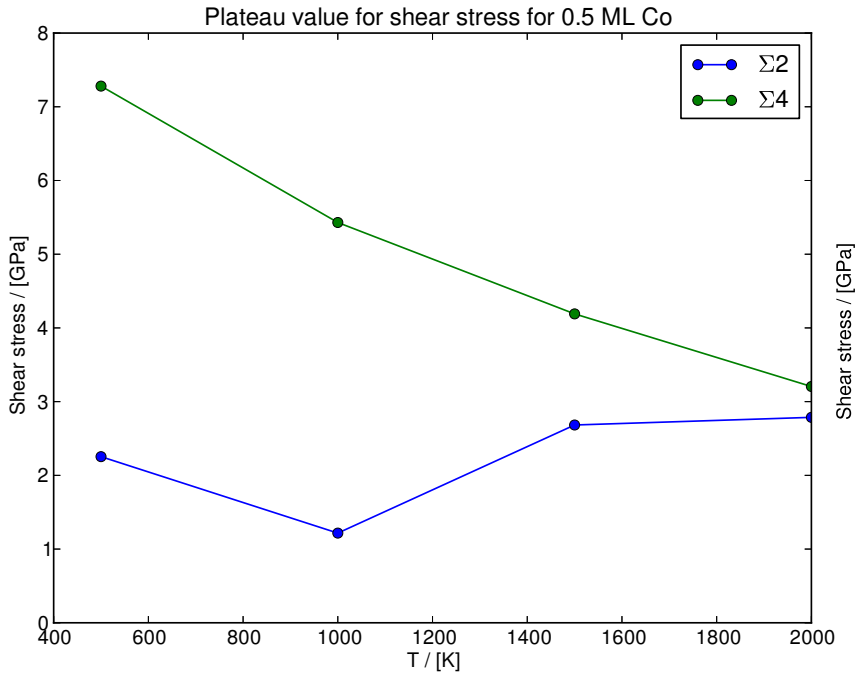
Results as function of T

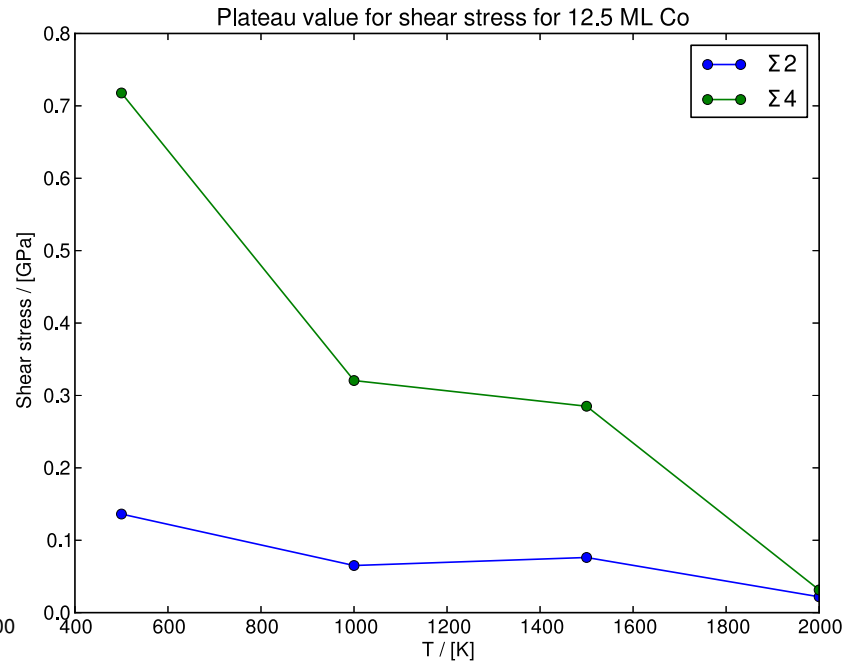


Observations

1. Co infiltration significantly facilitates gbs
2. A few layers, ~ 1 nm, of Co are required to facilitate gbs
3. Submonolayer Co segregation strengthens the grain boundary

Plateau stress, with and without Co film





- Significantly reduced plateau stresses with Co film:
  A few GPa $\rightarrow$ a few tenths of a GPa

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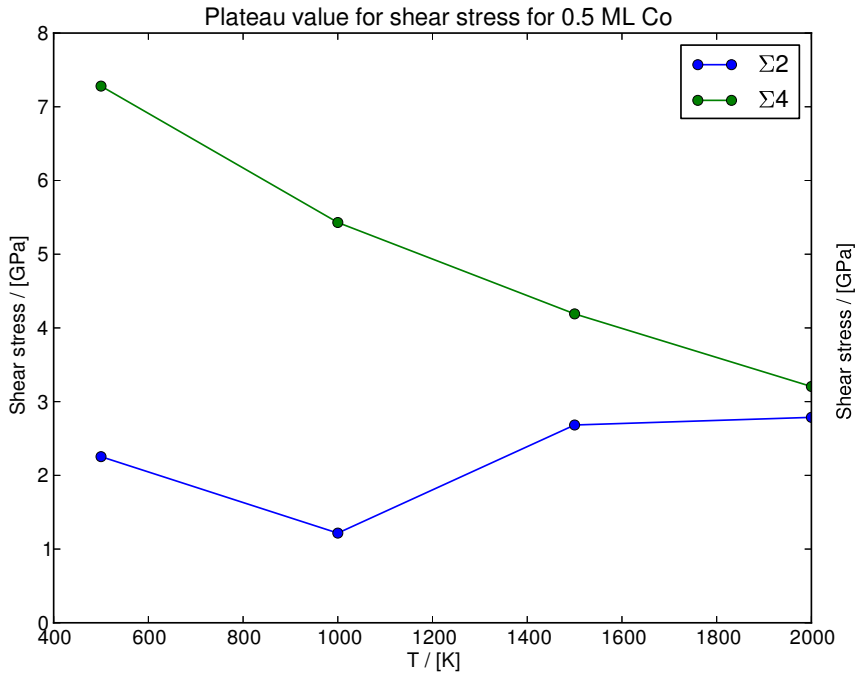
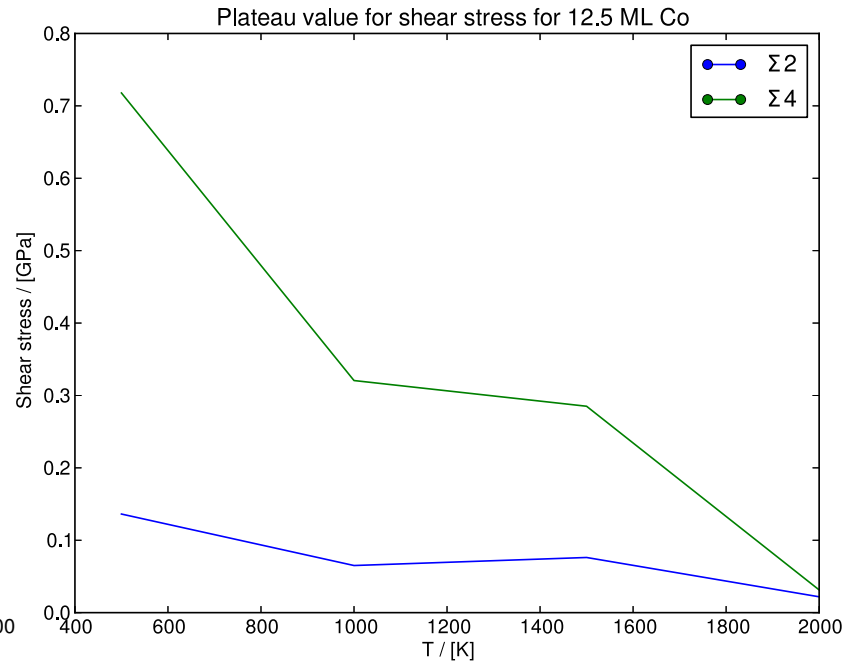
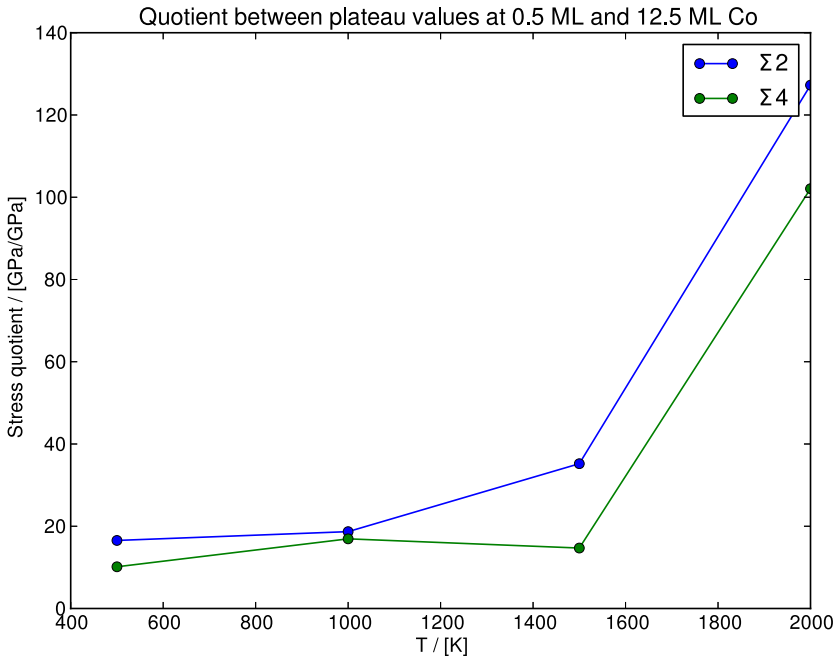




- Significantly reduced plateau stresses with Co film:
  A few GPa $\rightarrow$ a few tenths of a GPa
- Same plateau shear stress for Co film at 2000 K (Co liquid)

Quotient of stresses with and without Co film

Taking the quiotient of the previous stresses:



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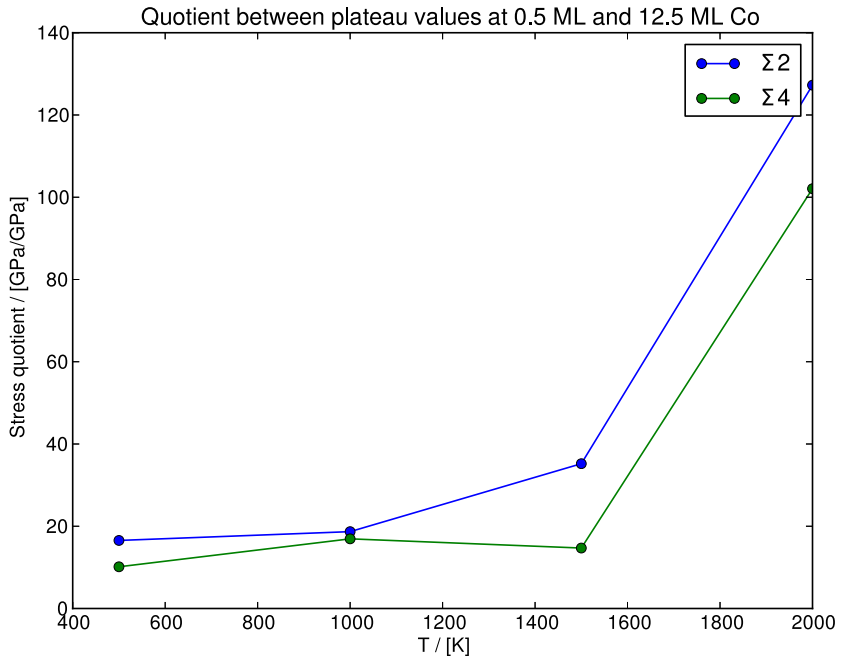

- ∼20 times lower shear stresses with 12 ML solid Co film compared to 0.5 ML Co

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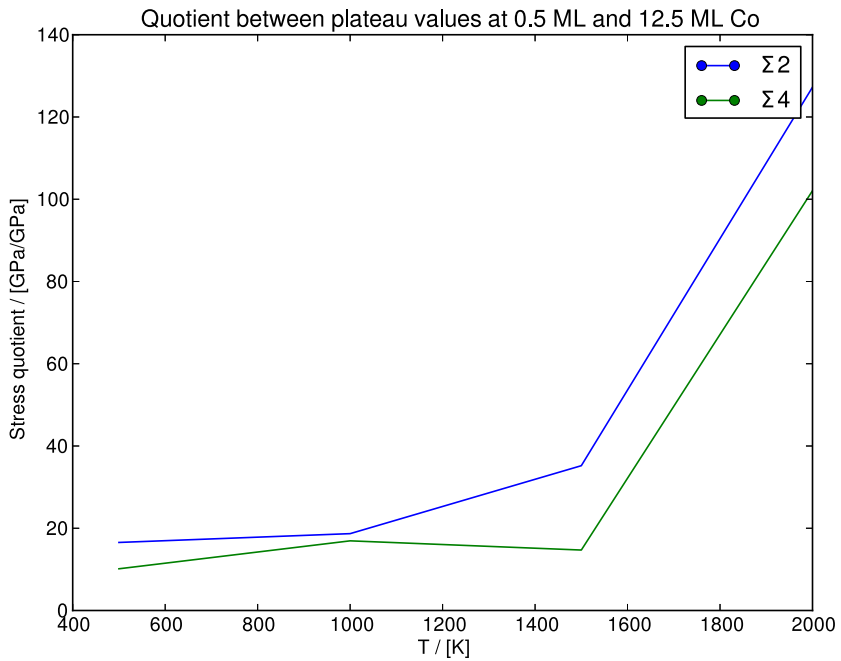


- ∼20 times lower shear stresses with 12 ML solid Co film compared to 0.5 ML Co
- ∼100 times lower shear stresses with 12 ML molten Co film compared to 0.5 ML Co

Summary

- Grain boundaries infiltrated by Co (12 monolayers) requires an order of magnitude smaller stresses to slide for $T < T_m^{\mathrm{Co}}$
- For $T = 2000\,\mathrm{K} > T_m^{\mathrm{Co}}$ the stresses are two orders of magnitude smaller
- A film of 6 Co layers ($\sim$1 nm) is enough to facilitate gbs

Infiltration of Co into WC/WC grain boundaries: A work in progress

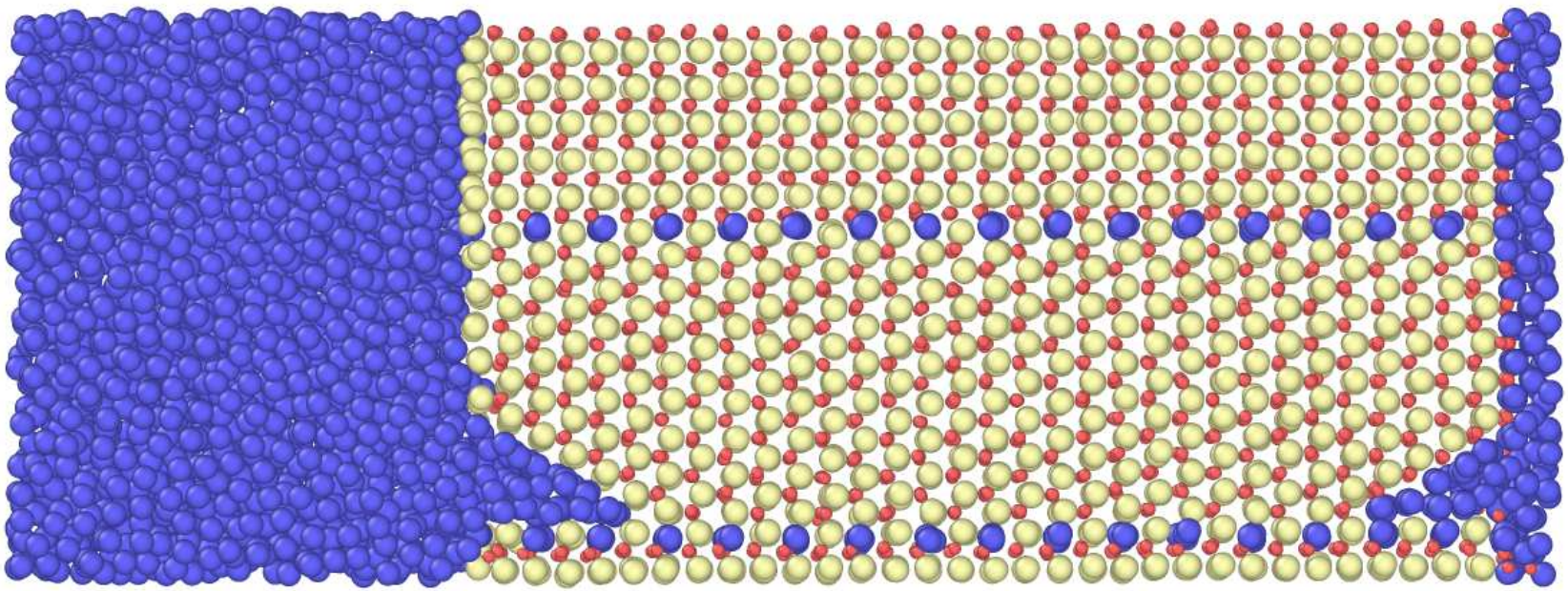
Infiltration of Co into Σ2 grain boundary

System

- Bicrystal with WC/WC grain boundary
- Reservoir of Co for infiltration
- Wedge in the WC/WC grain boundary filled with Co to aid infiltration

Infiltration of Co into Σ2 grain boundary

System



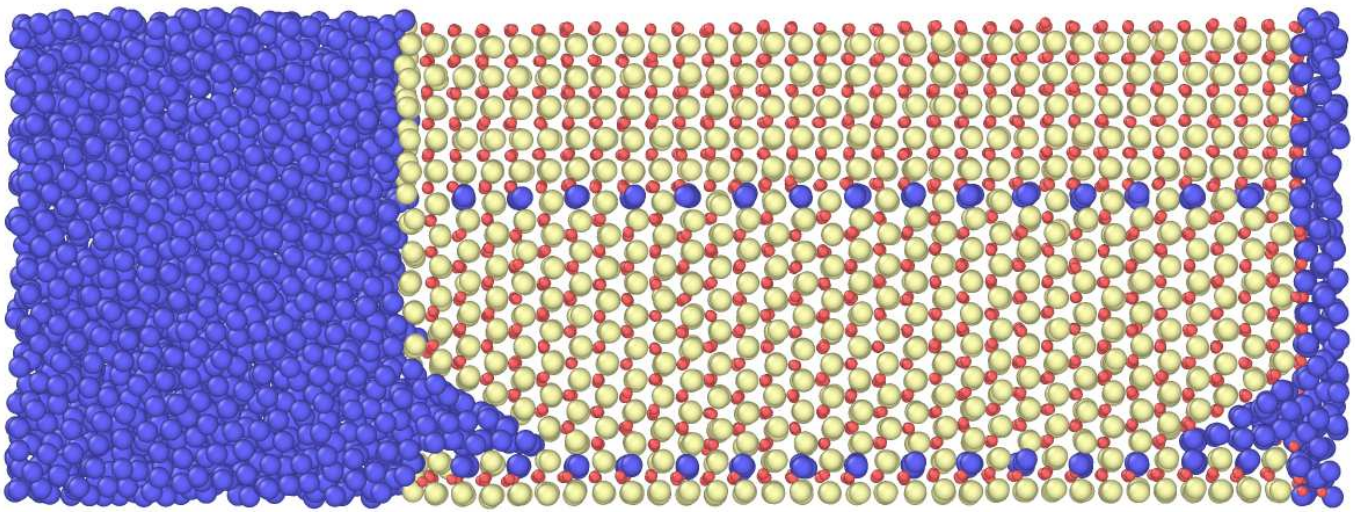
Infiltration of Co into Σ2 grain boundary

Simulation method

- Constant strain rate of 0.01 ns^{-1} perpendicular to grain boundary
- Zero pressure in grain boundary plane
- 2000 K
- Periodic boundary conditions in all directions

Infiltration of Co into Σ2 grain boundary

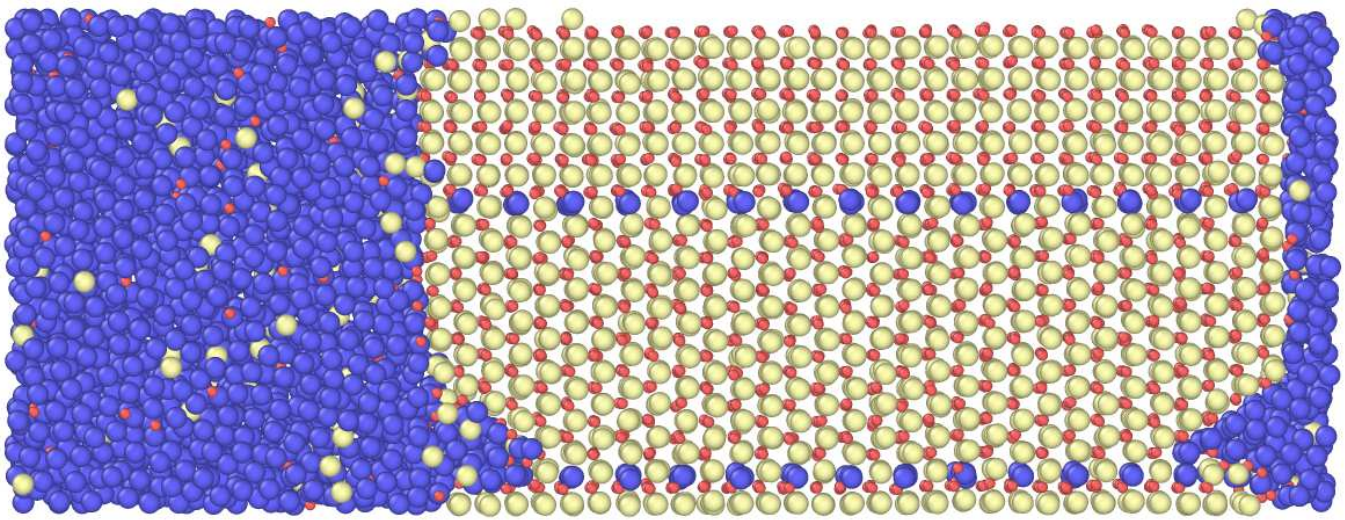
Constant strain rate



0 ns

Infiltration of Co into Σ2 grain boundary

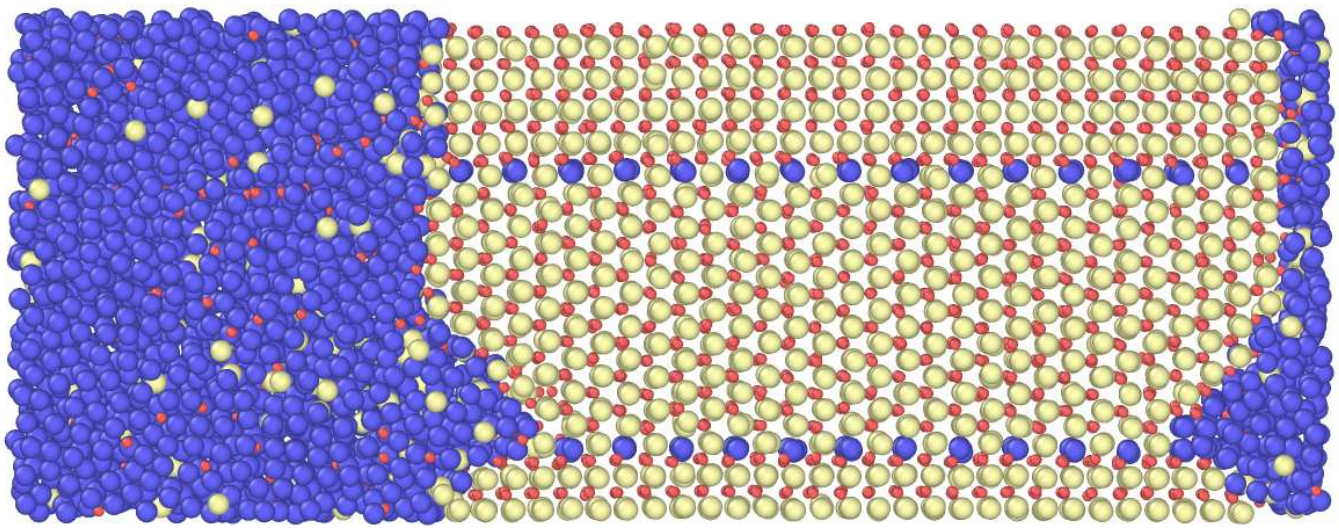
Constant strain rate



1.5 ns

Infiltration of Co into Σ2 grain boundary

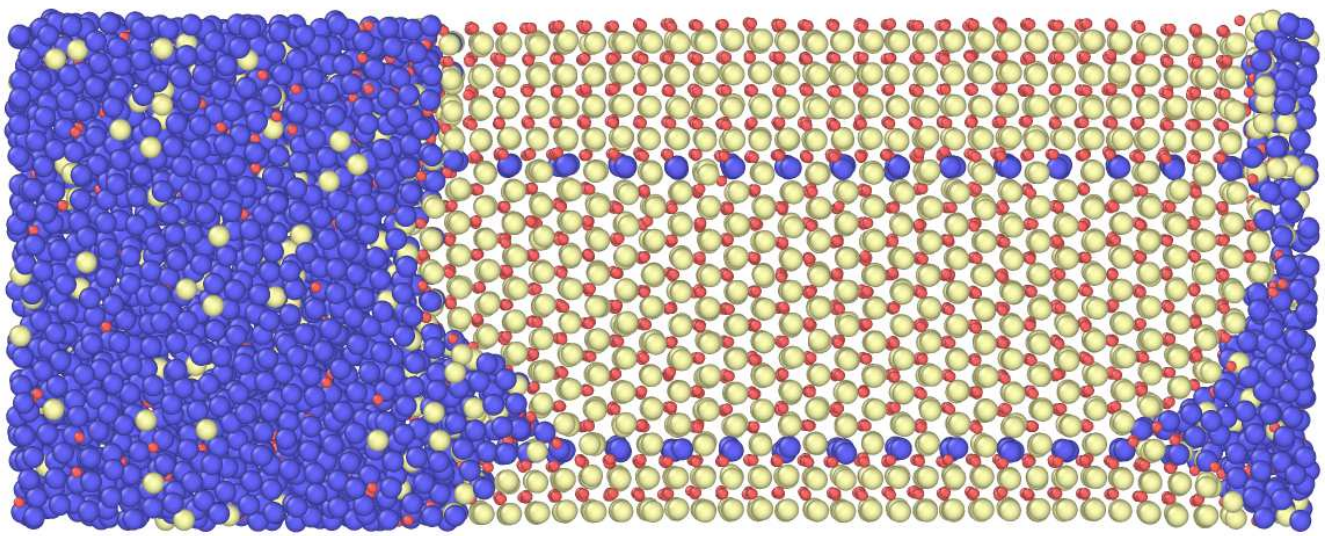
Constant strain rate



3 ns

Infiltration of Co into Σ2 grain boundary

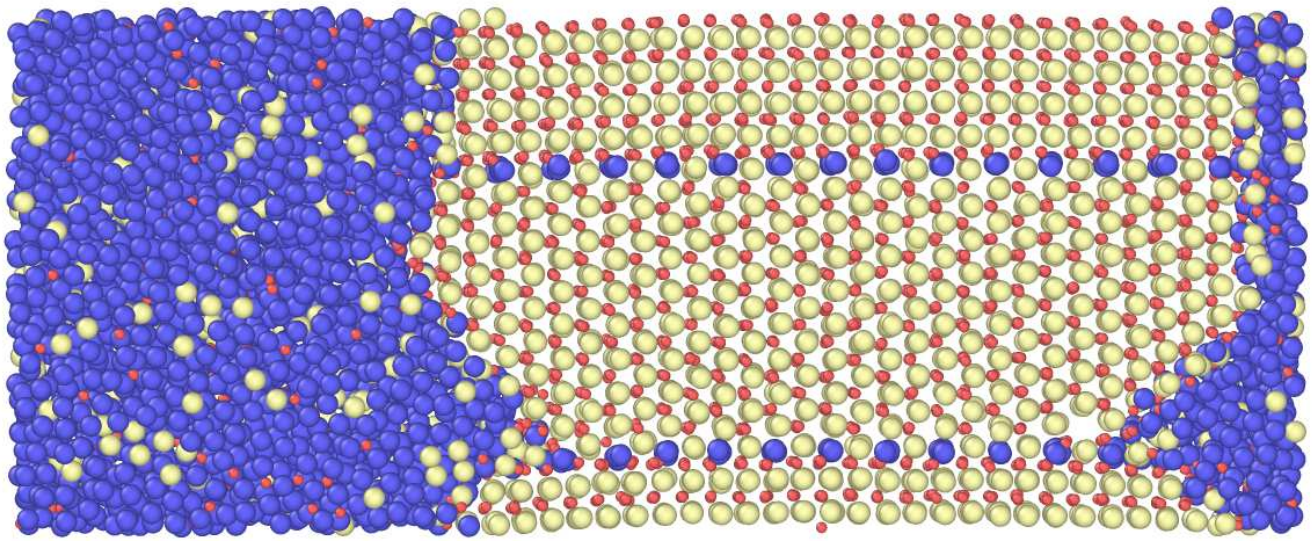
Constant strain rate



4.5 ns

Infiltration of Co into Σ2 grain boundary

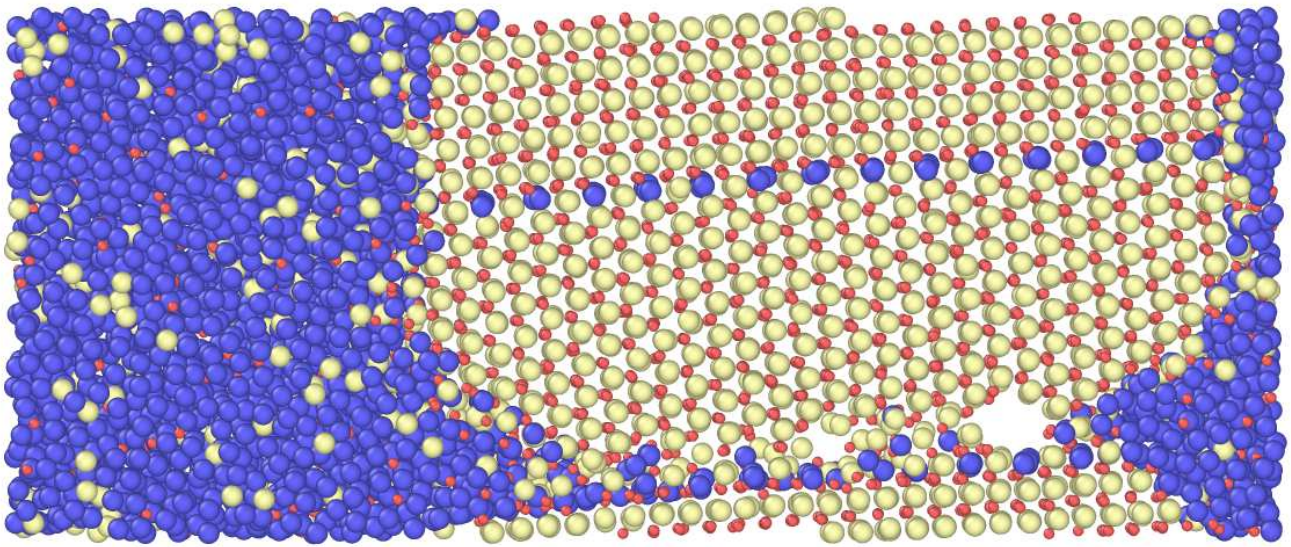
Constant strain rate



6 ns

Infiltration of Co into Σ2 grain boundary

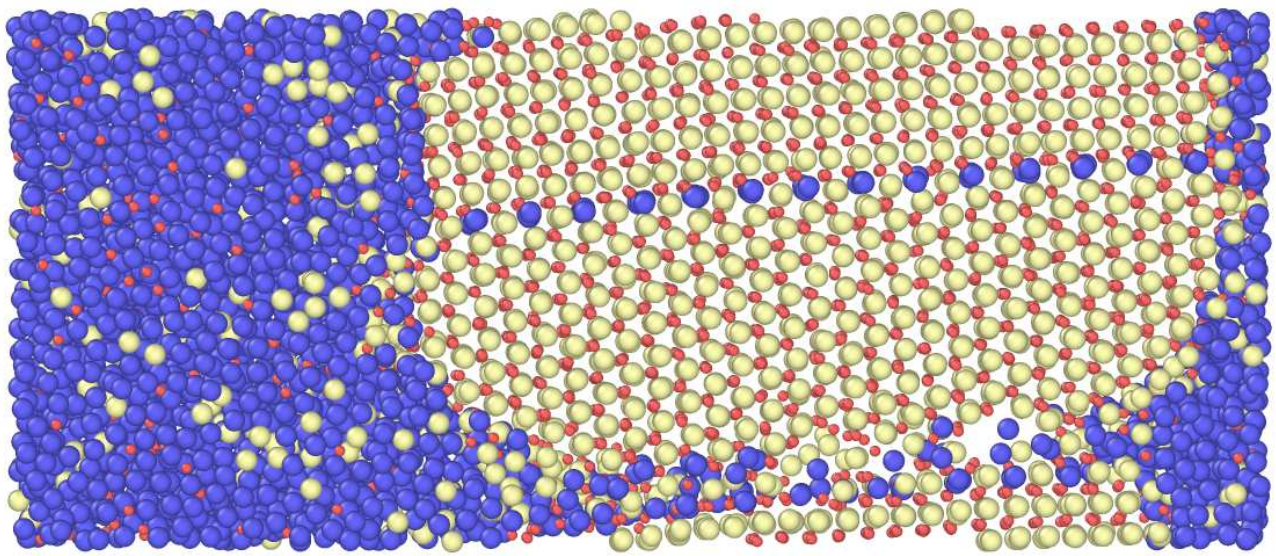
Constant strain rate



7.5 ns

Infiltration of Co into Σ2 grain boundary

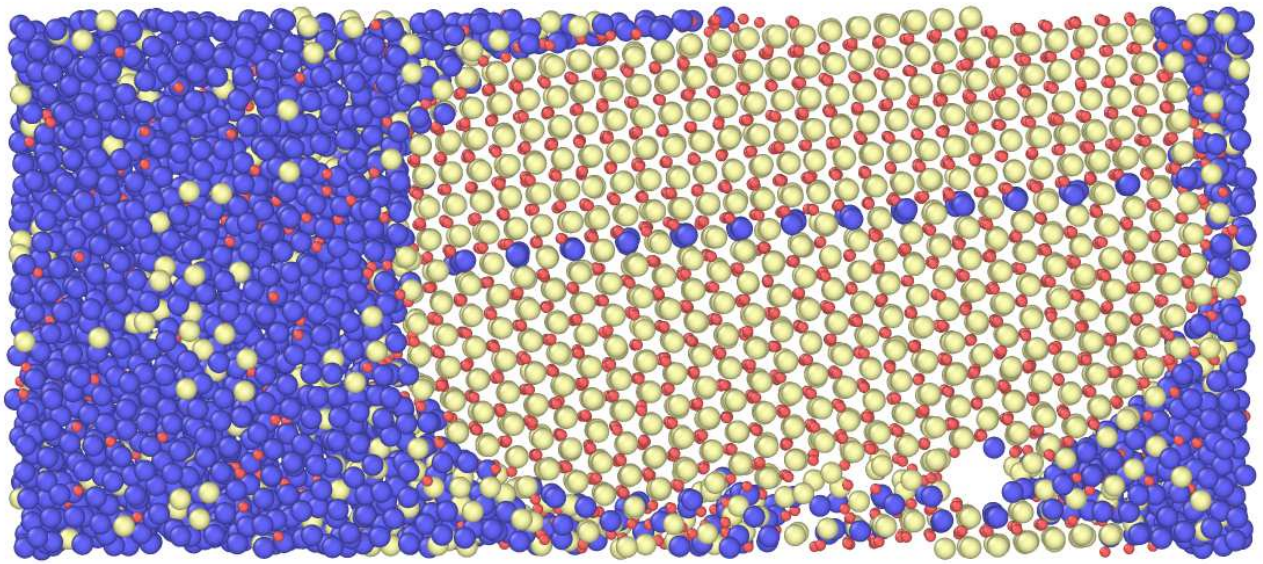
Constant strain rate



9 ns

Infiltration of Co into Σ2 grain boundary

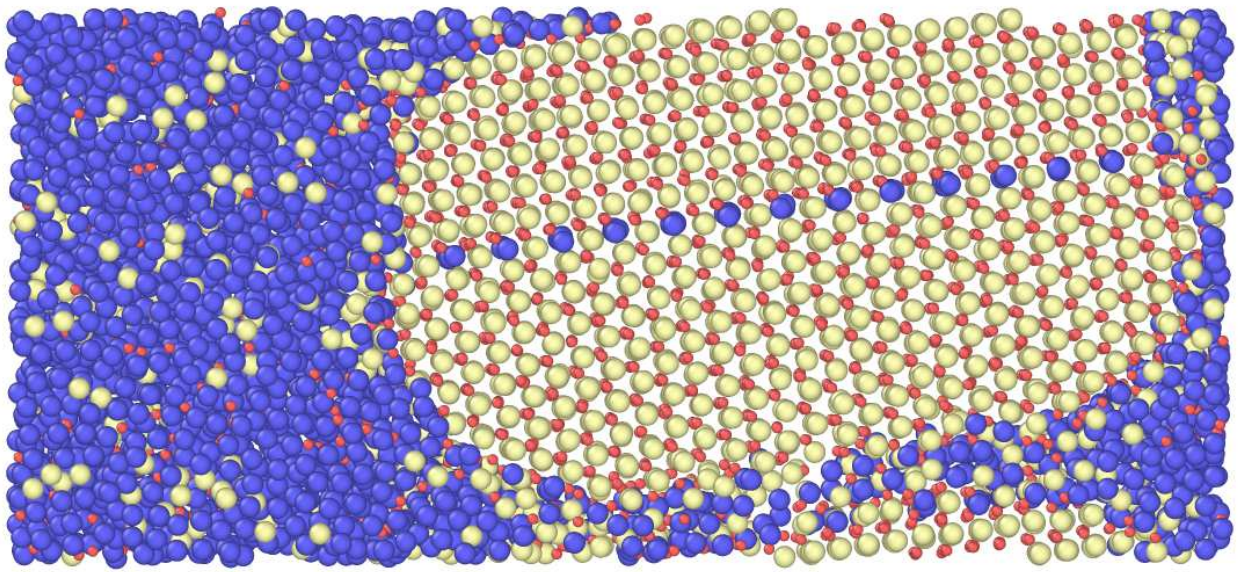
Constant strain rate



10.5 ns

Infiltration of Co into Σ2 grain boundary

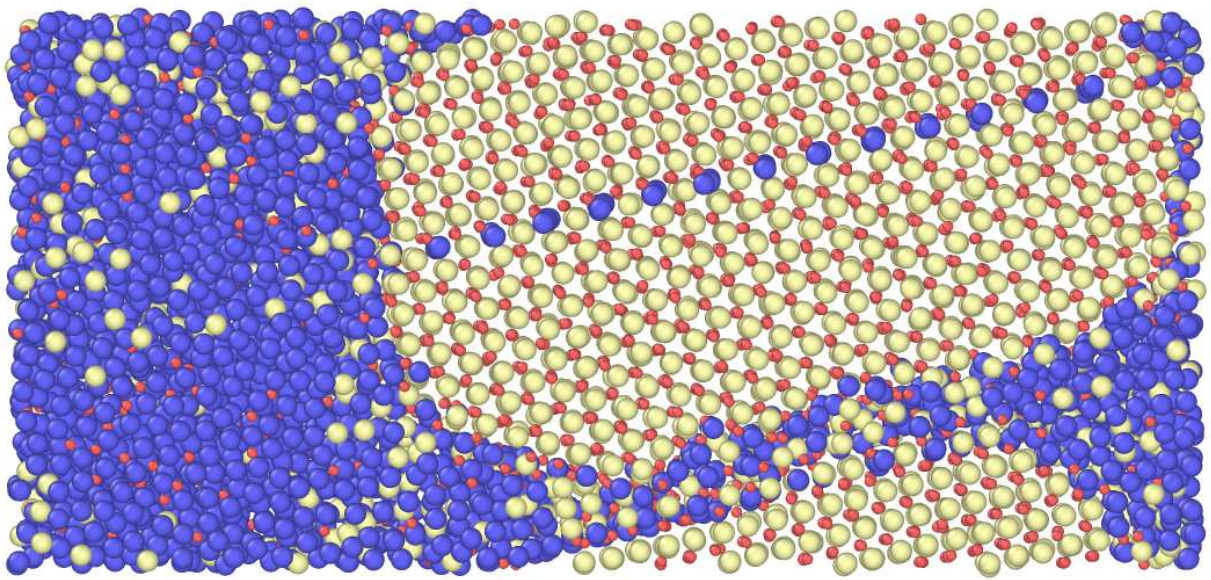
Constant strain rate



12 ns

Infiltration of Co into Σ2 grain boundary

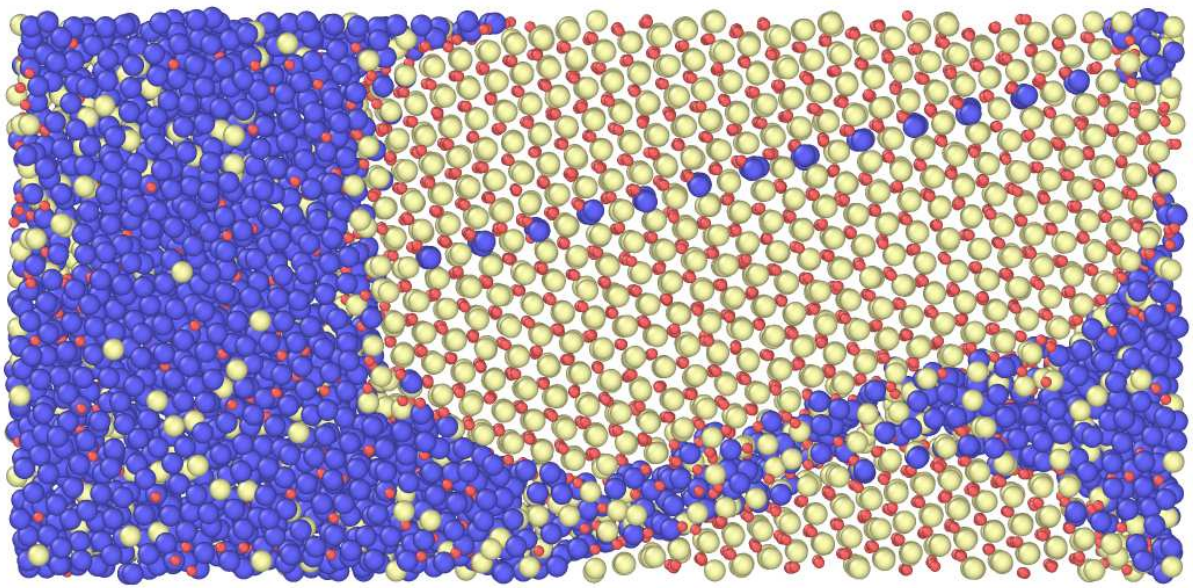
Constant strain rate



13.5 ns

Infiltration of Co into Σ2 grain boundary

Constant strain rate



15 ns

Infiltration of Co into Σ2 grain boundary

Constant strain rate

- Peak stress matches reference simulation without Co reservoir and wedge, $\sim$ 25 GPa
- Grain boundary separates before Co infiltrates
- Need larger time-scales to see infiltration
- W and C in WC/Co interfaces diffuse into the Co reservoir:
  Due to a driving force from the fitting of the potential

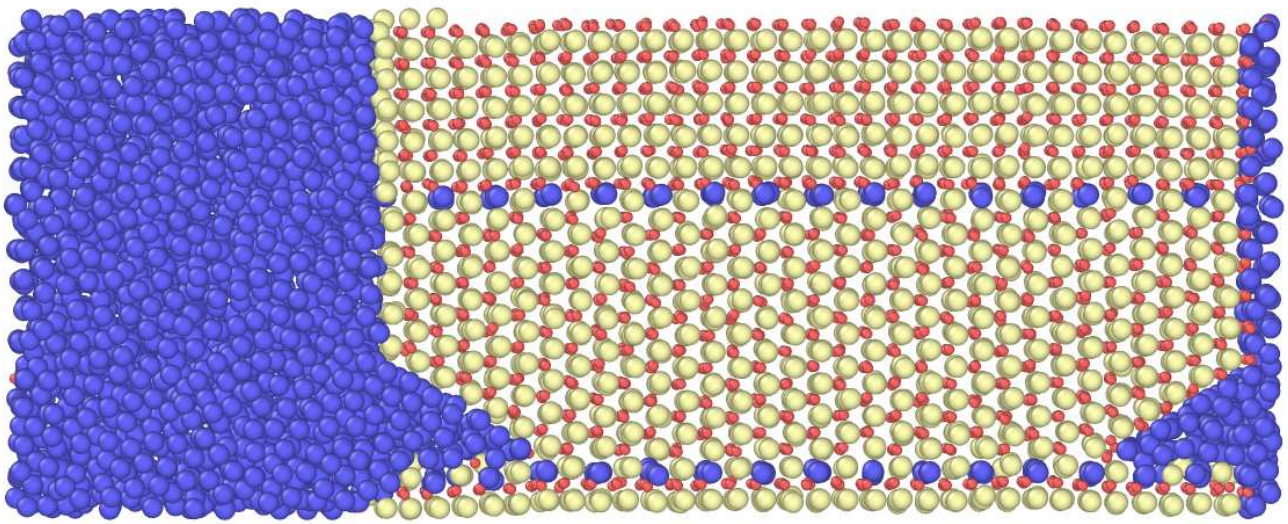
Infiltration of Co into Σ2 grain boundary

Simulation method

- Constant stress perpendicular to grain boundary
- Zero pressure in grain boundary plane
- 2000 K
- Periodic boundary conditions in all directions

Infiltration of Co into Σ2 grain boundary

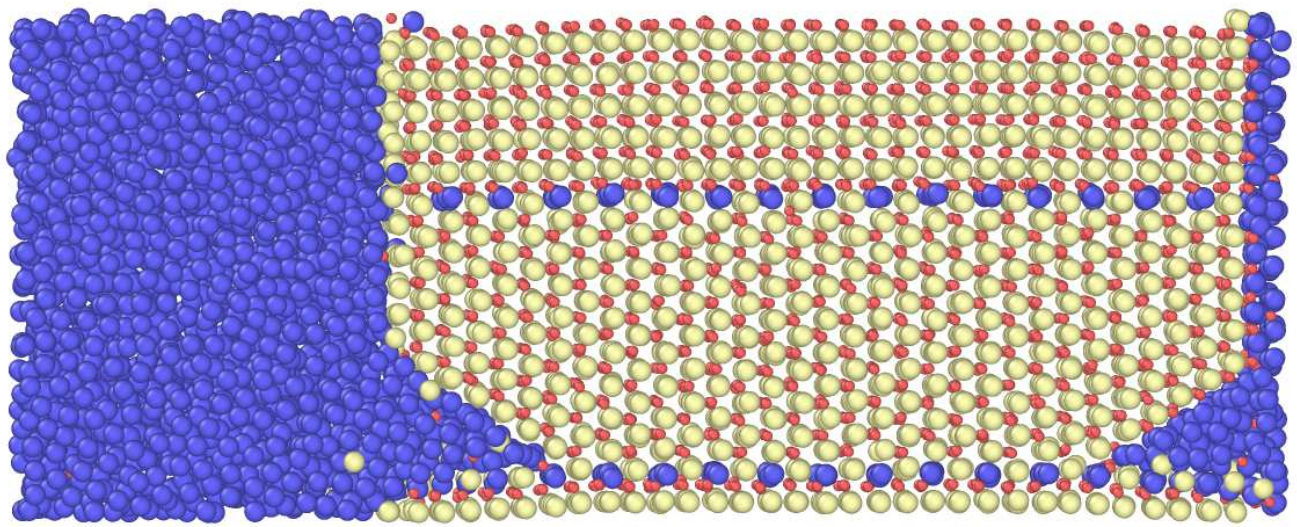
Constant stress ($\sim$ 20 GPa)



0 ns

Infiltration of Co into Σ2 grain boundary

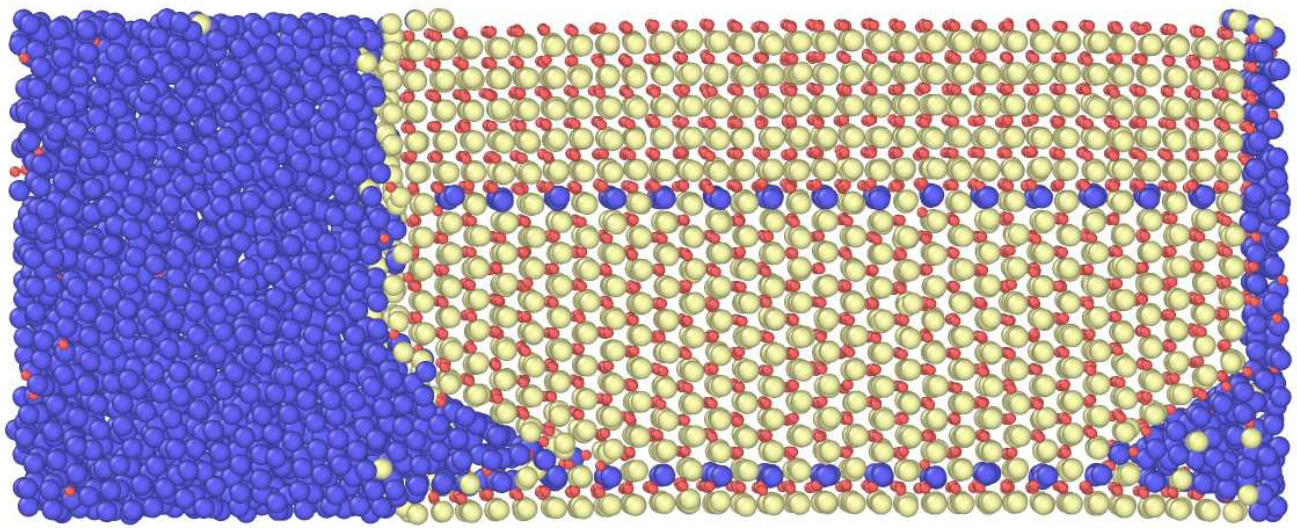
Constant stress ($\sim$ 20 GPa)



0.15 ns

Infiltration of Co into Σ2 grain boundary

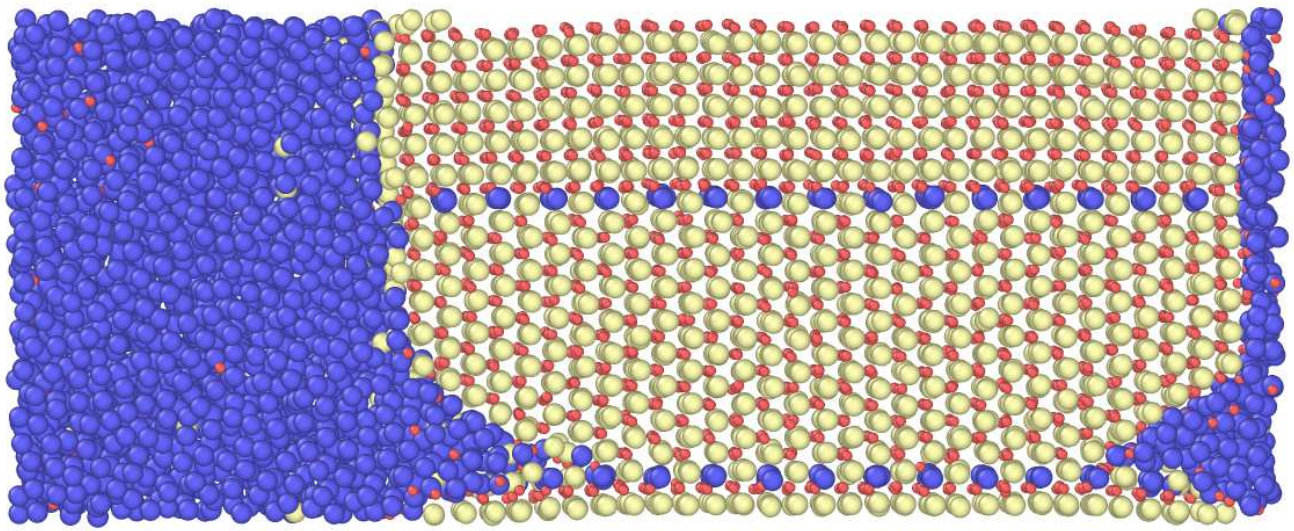
Constant stress ($\sim$ 20 GPa)



0.3 ns

Infiltration of Co into Σ2 grain boundary

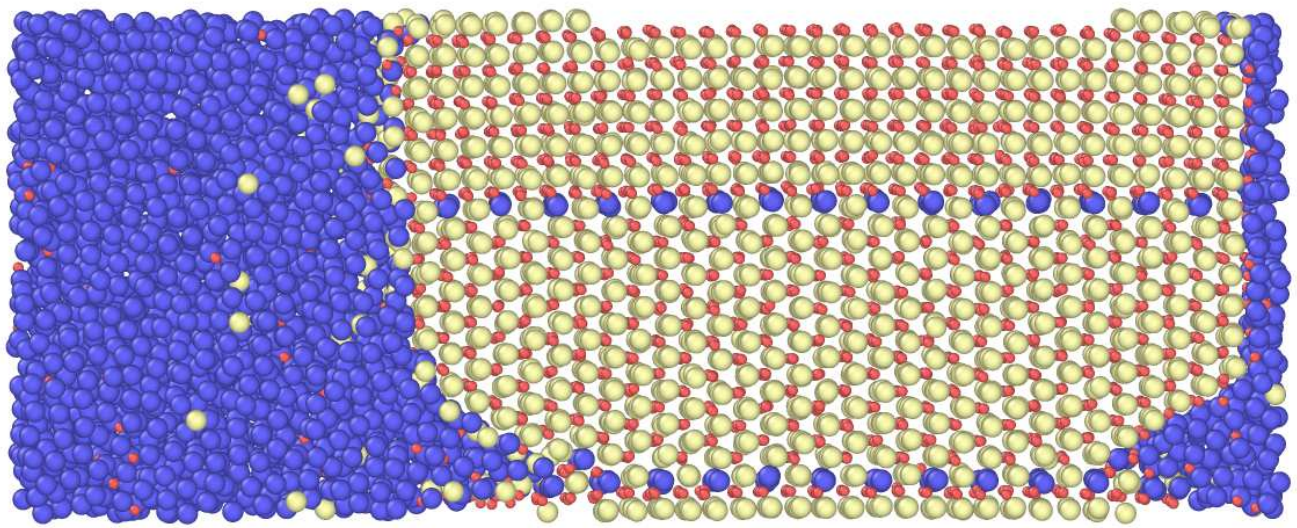
Constant stress ($\sim$ 20 GPa)



0.45 ns

Infiltration of Co into Σ2 grain boundary

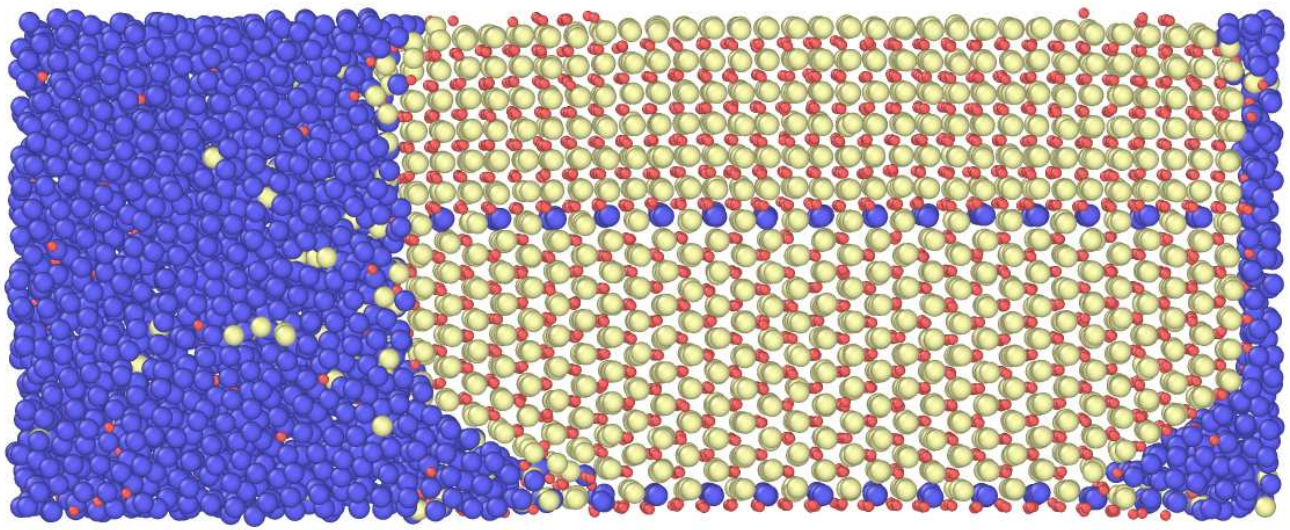
Constant stress ($\sim$ 20 GPa)



0.6 ns

Infiltration of Co into Σ2 grain boundary

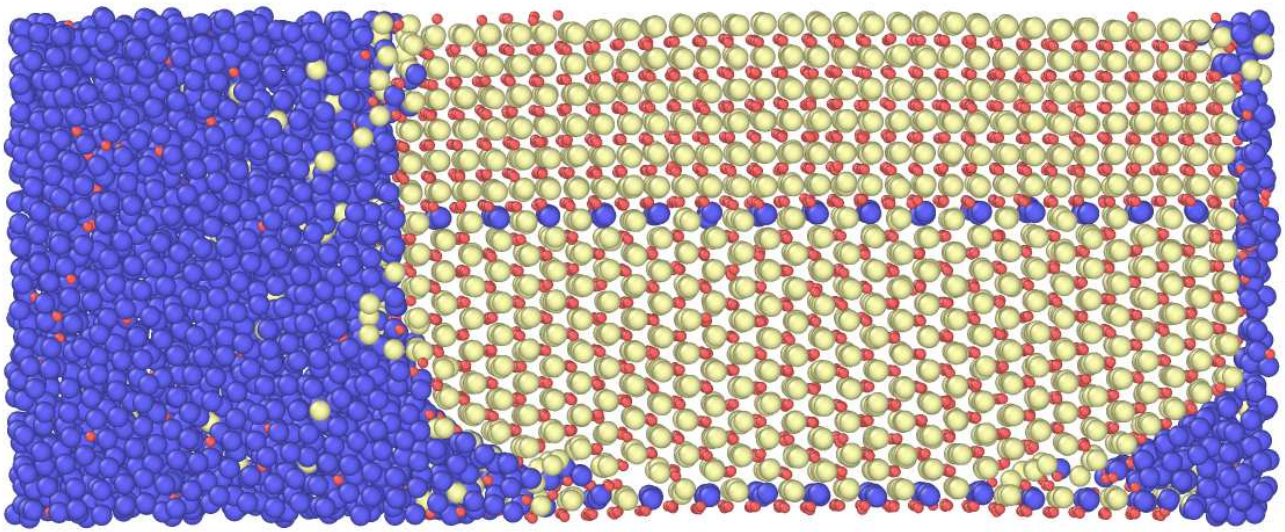
Constant stress ($\sim$ 20 GPa)



0.75 ns

Infiltration of Co into Σ2 grain boundary

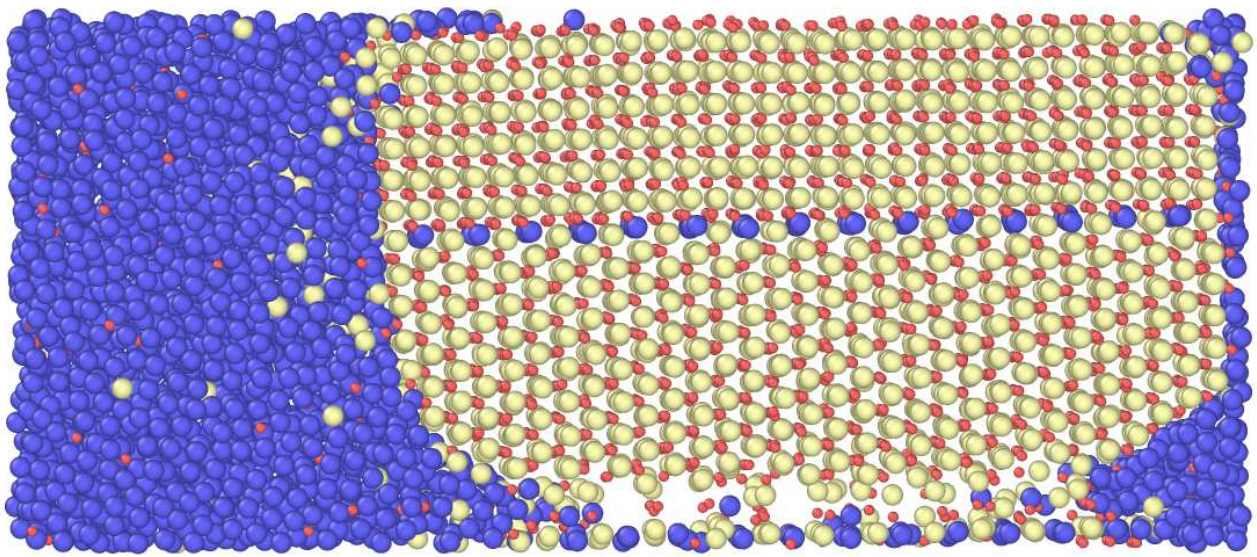
Constant stress ($\sim$ 20 GPa)



0.9 ns

Infiltration of Co into Σ2 grain boundary

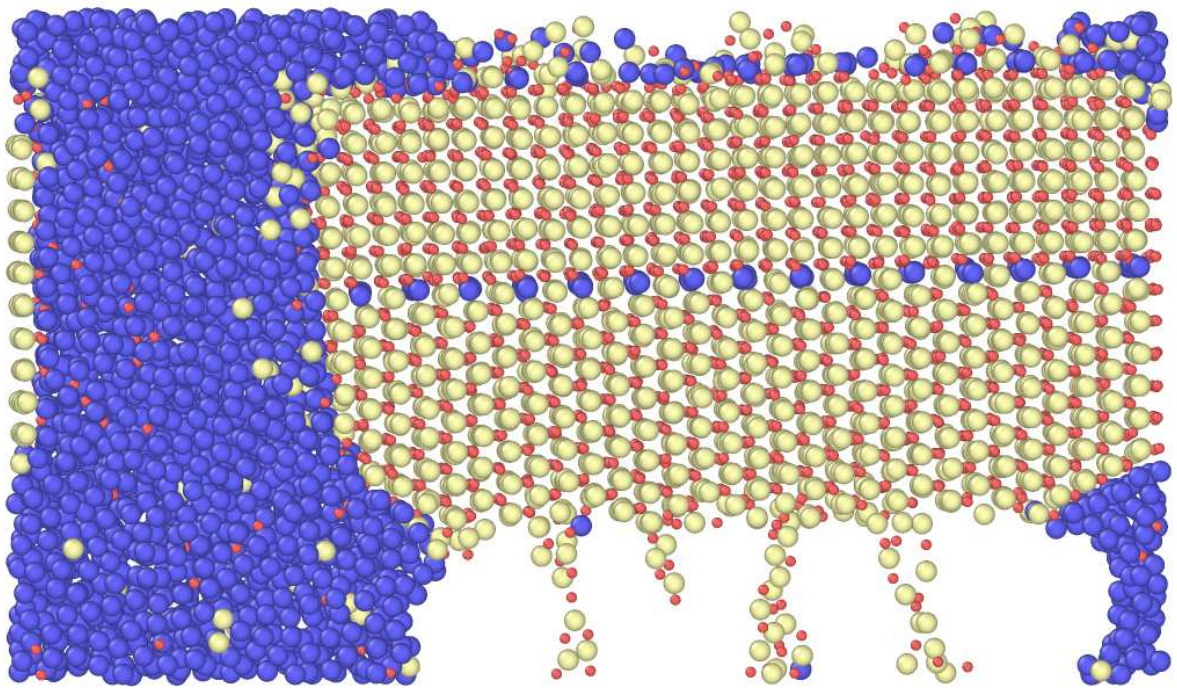
Constant stress ($\sim$ 20 GPa)



0.92 ns

Infiltration of Co into Σ2 grain boundary

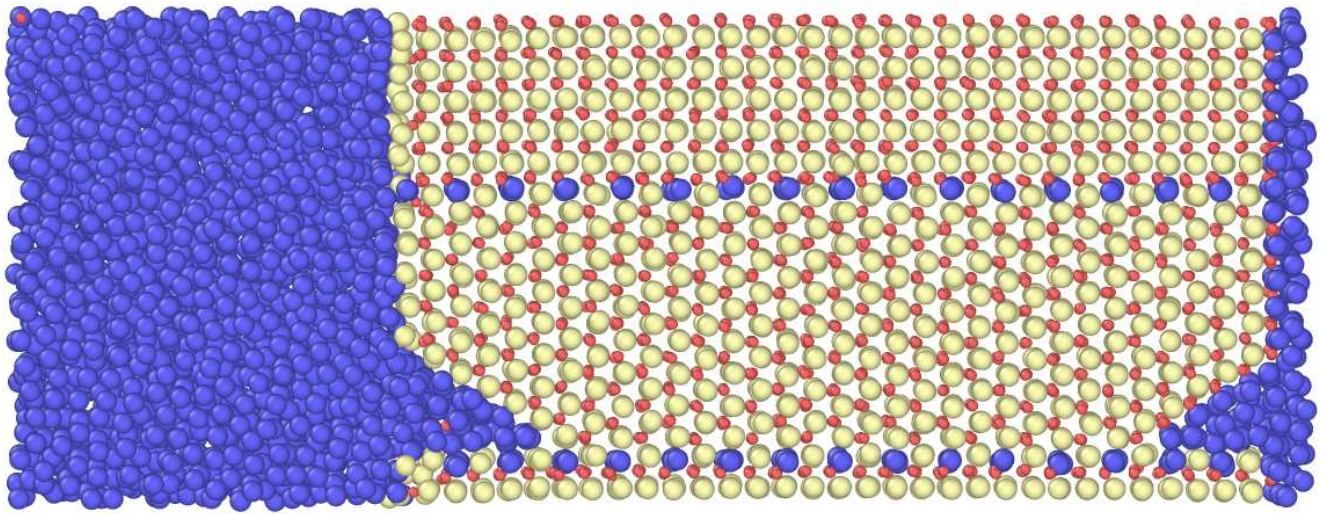
Constant stress ($\sim$ 20 GPa)



0.925 ns

Infiltration of Co into Σ2 grain boundary

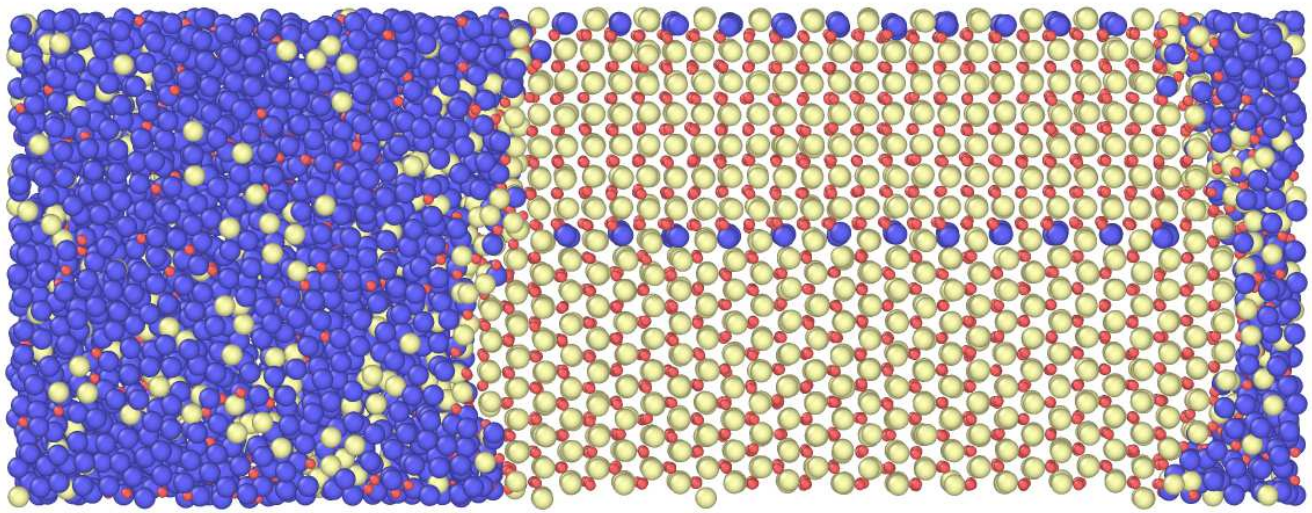
Constant stress ($\sim$ 10 GPa)



0 ns

Infiltration of Co into Σ2 grain boundary

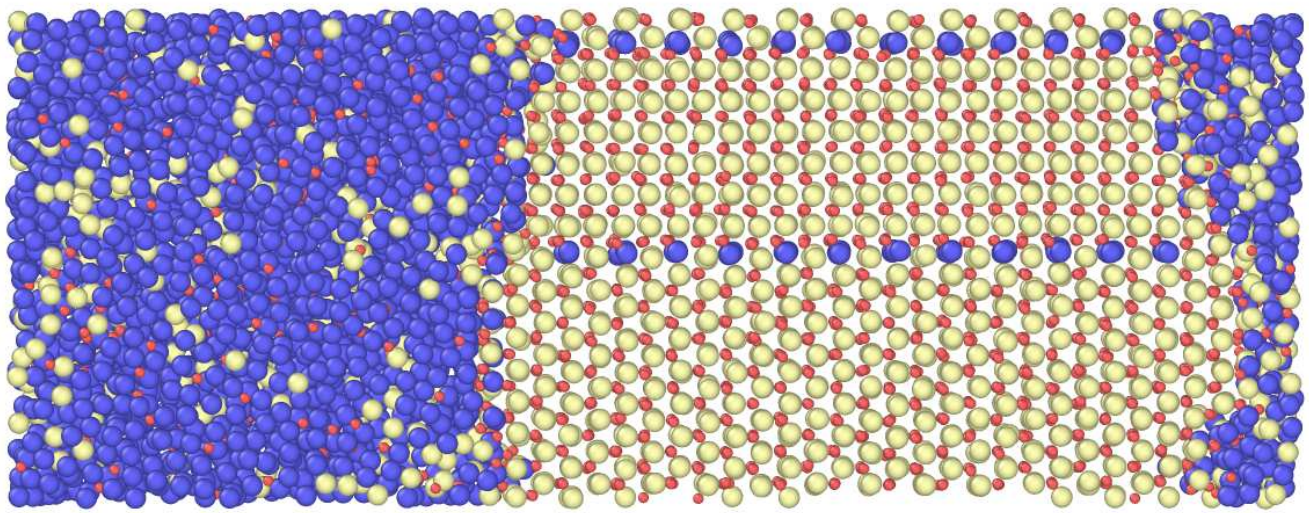
Constant stress ($\sim$ 10 GPa)



45 ns

Infiltration of Co into Σ2 grain boundary

Constant stress ($\sim$ 10 GPa)



75 ns

Infiltration of Co into Σ2 grain boundary

Conclusion

- Molecular dynamics cover to small time scales to see infiltration
- Need to force the infiltration of Co
- $\Rightarrow$ Monte Carlo simulations

Summary

Infiltration

- MD cover to small time scales to see infiltration in WC-Co
- Diffusion of W and C into Co can be studied using MD

Grain boundary sliding

- Grain boundaries infiltrated by Co (12 monolayers) requires an order of magnitude smaller stresses to slide for $T < T_m^{\mathrm{Co}}$
- For $T = 2000\,\mathrm{K} > T_m^{\mathrm{Co}}$ the stresses are two orders of magnitude smaller
- A film of 6 Co layers ($\sim$1 nm) is enough to facilitate gbs

Outlook

- Further investigate Co infiltration, maybe use Monte Carlo to force Co into the grain boundary.

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- Further investigate Co infiltration, maybe use Monte Carlo to force Co into the grain boundary.

Thank you for listening!