

# Solutions for metal cutting

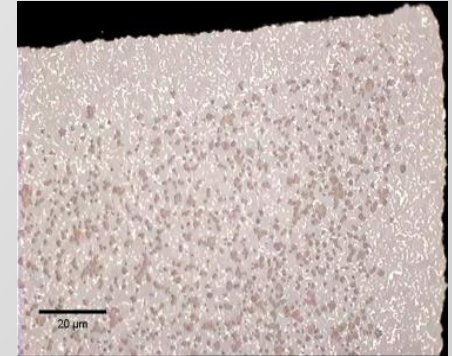
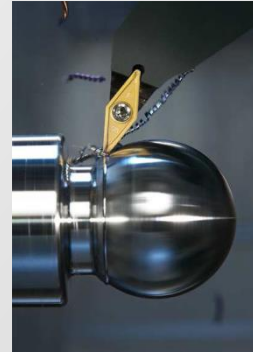
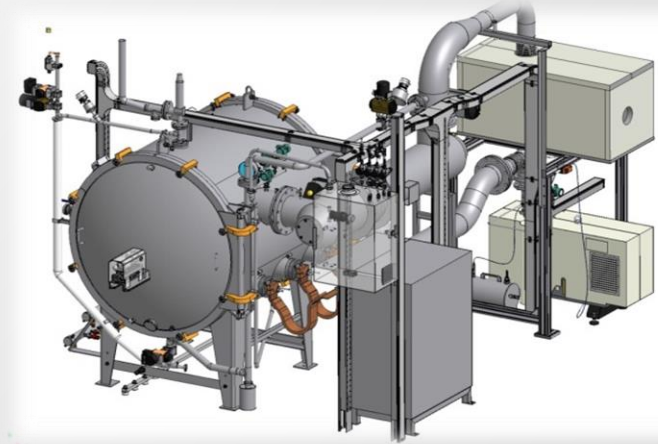
Applications of thermodynamic calculations

Henrik Strandlund

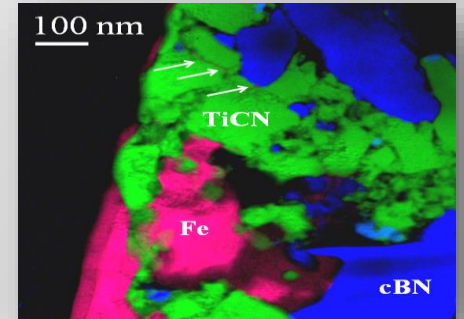
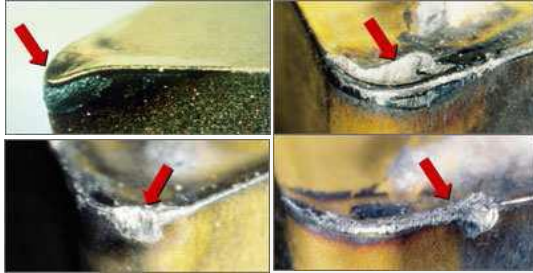
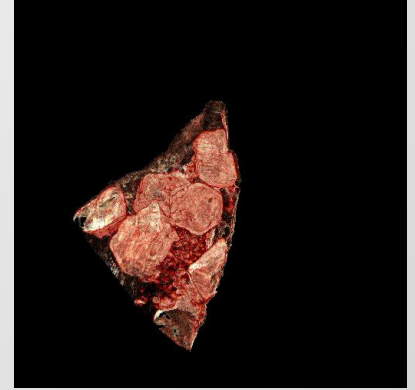
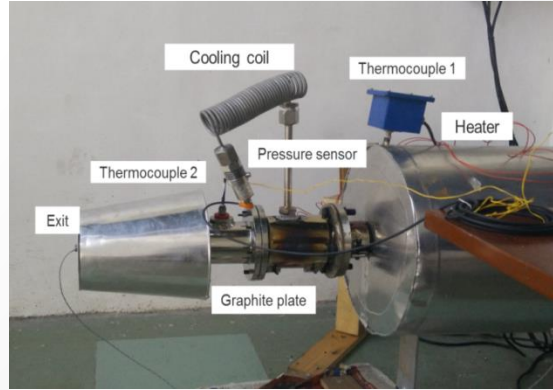


# Applications

- Machining dynamics
- Metal cutting
- ***Wear of inserts***
- ***Manufacturing processes***
- Solid mechanics
- ***Mechanical properties***
- ***Thermodynamic properties***
- ***Microstructure in materials***
- ***Defects in materials***



# Generating input data and verification of results

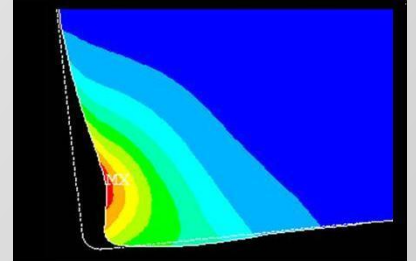
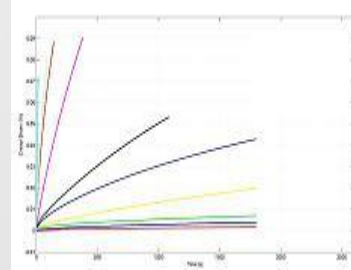
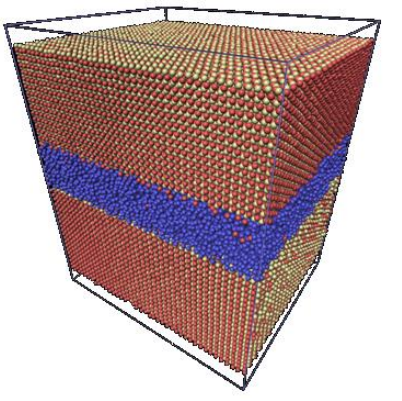




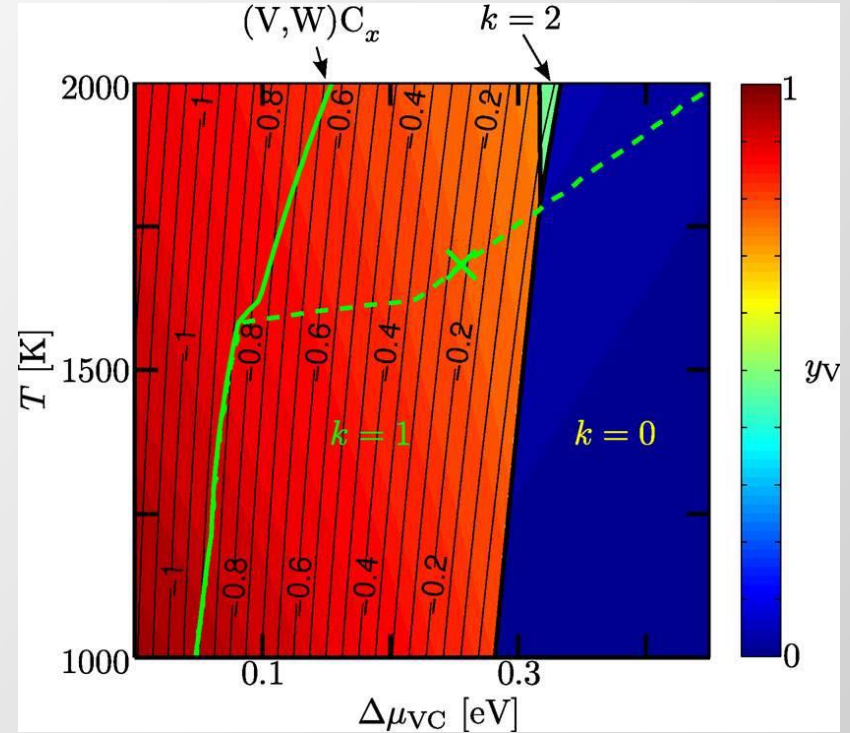
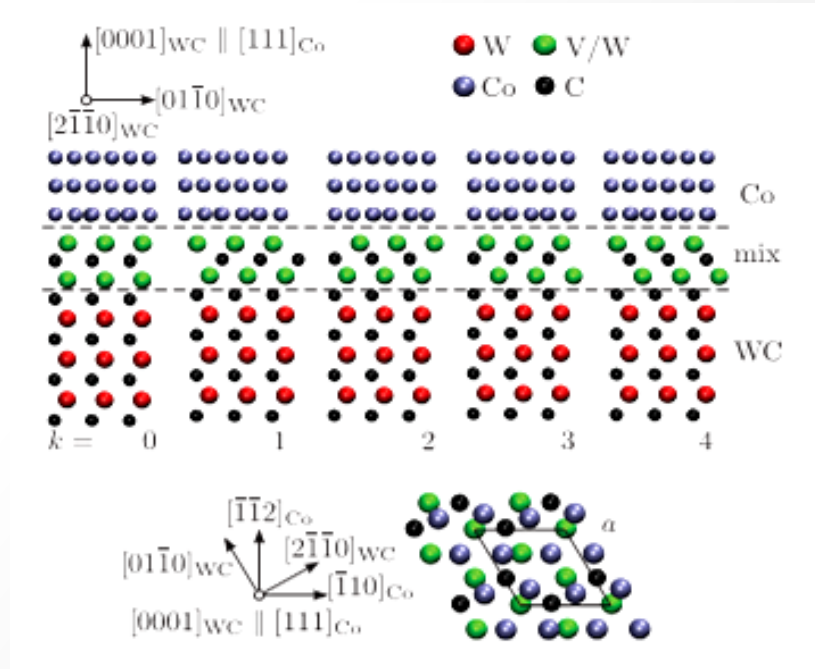
# Wear of inserts

## Predicting plastic deformation

Fundamental atomistic simulations, thermodynamic calculations and measurements to generate input to models



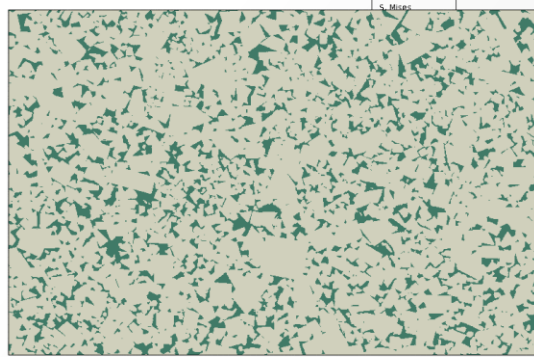
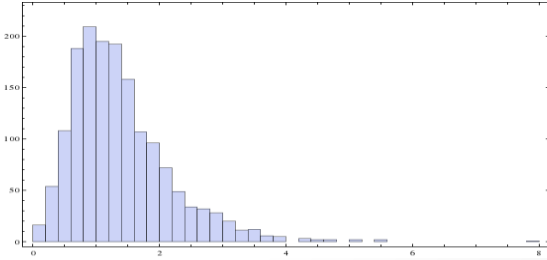
# Thermodynamics properties and defects



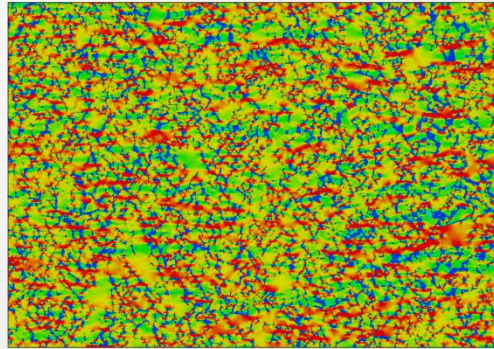
S. A. E. Johansson and G. Wahnström, Phys Rev B 86, 035403 (2012)

# Microstructure in materials and mechanical properties

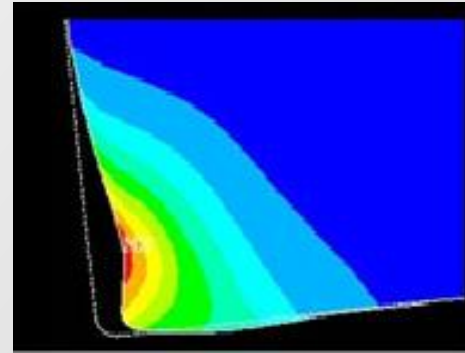
## Microstructural FEM of plastic deformation



Microstructure before  
Deformation (SEM image)



Simulated deformed  
microstructure



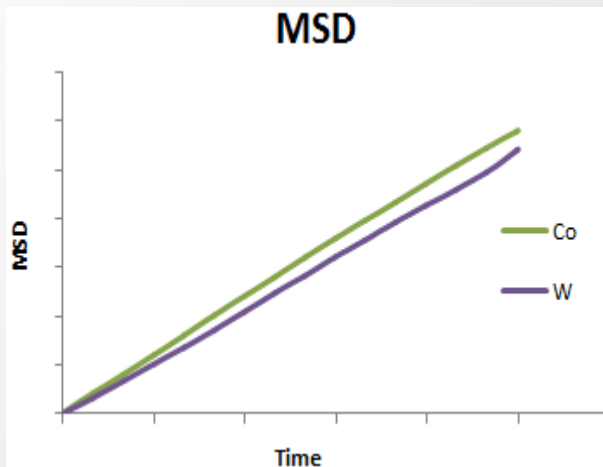
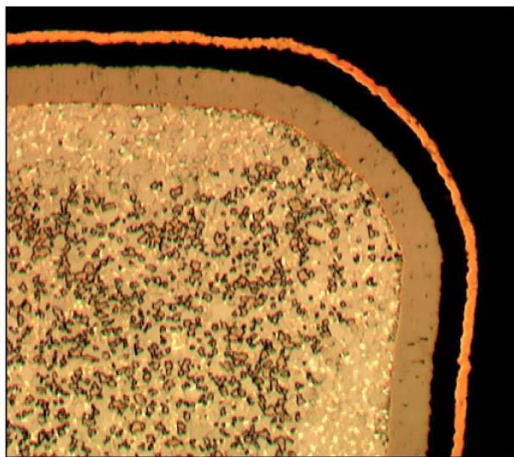
Simulated macroscopic  
deformation



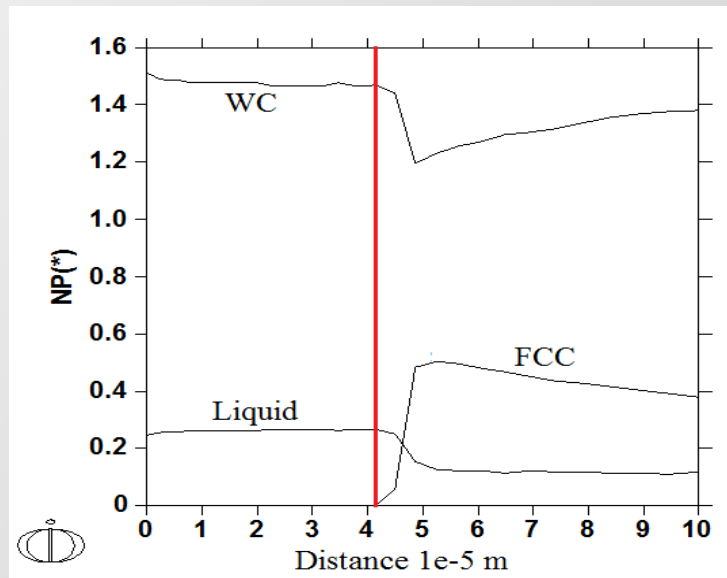
# Microstructure in materials and mechanical properties

## Gradient formation in cemented carbides

Atomistic mobilities in liquid state, Ab-initio MD simulations



Depth of the gradient



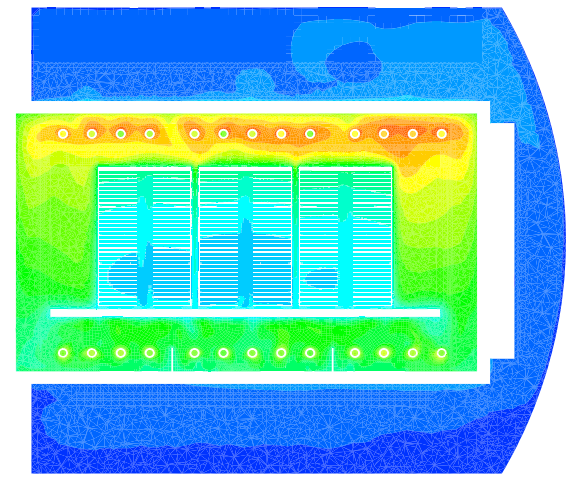
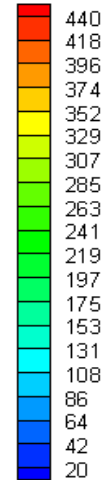
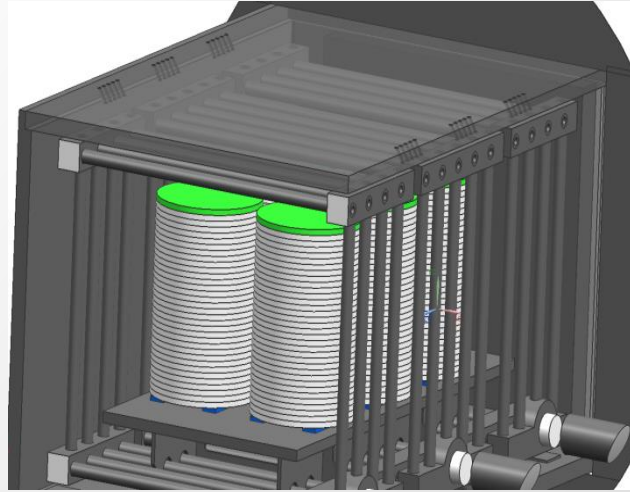
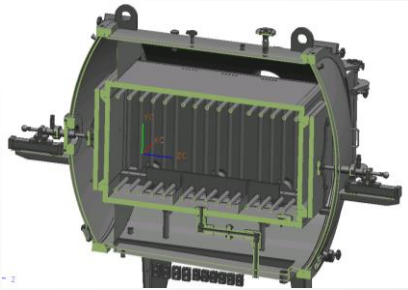
M Wahlbrül, Master Thesis, 2014

# Properties of manufacturing processes

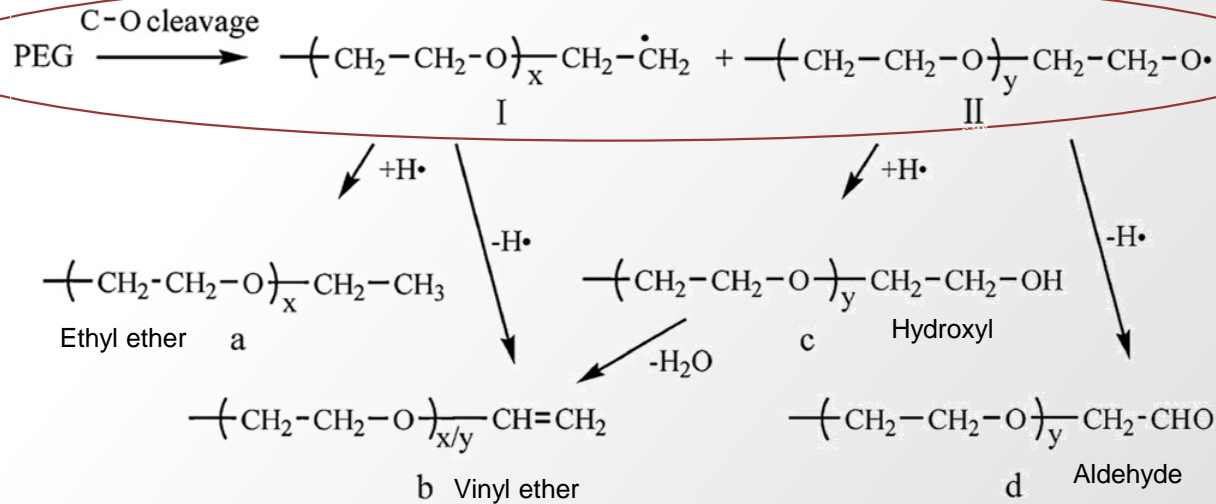
## Otimization of sintering processes and furnaces

Optimizing equipment and processes by simulating and studying gas and temperature distribution

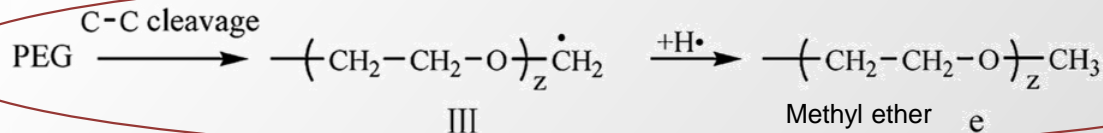
### Simulations of debinding



# Decomposition of the binder (PEG)



At low Temp (Onset of reaction)



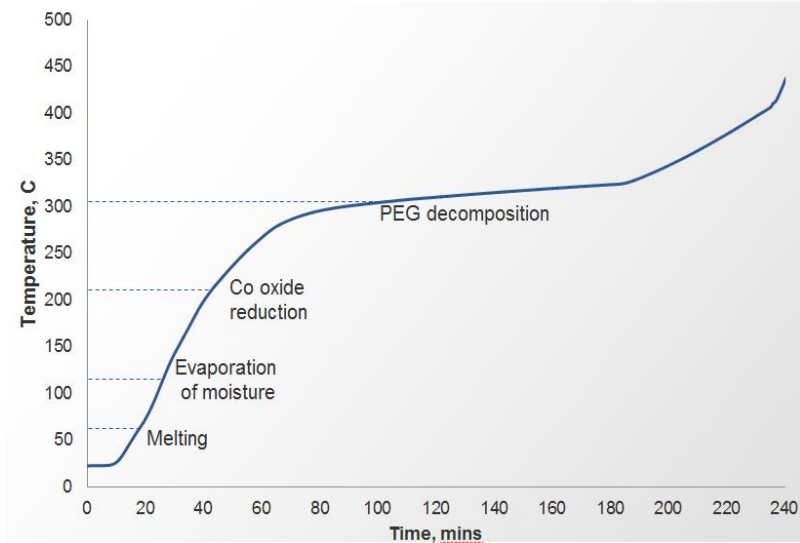
At high Temp (above 200 °C)

Scheme 1. The decomposition pathway of PEG.

# Decomposition of the binder (PEG)

Group name	Product series	Molecular weight	Comp (%)
A	$\text{CH}_3-(\text{O}-\text{CH}_2-\text{CH}_2)_n-\text{O}-\text{CH}_2-\text{CH}_2-\text{OH}$	120-516	0.5-2.5
B	$\text{CH}_3-(\text{O}-\text{CH}_2-\text{CH}_2)_n-\text{O}-\text{CH}_3$	90-354	
C	$\text{HO}-\text{CH}_2-\text{CH}_2-(\text{O}-\text{CH}_2-\text{CH}_2)_n-\text{OH}$	102-546	
D	$\text{OHC}-\text{CH}_2-(\text{O}-\text{CH}_2-\text{CH}_2)_n-\text{OH}$	100-544	
E	$\text{CH}_3-\text{CH}_2-(\text{O}-\text{CH}_2-\text{CH}_2)_n-\text{O}-\text{CH}_3$	100-408	1-3.1
F	$\text{CH}_2=\text{CH}-(\text{O}-\text{CH}_2-\text{CH}_2)_n-\text{O}-\text{CH}_3$	102-410	
G	$\text{CH}_3-\text{CH}_2-(\text{O}-\text{CH}_2-\text{CH}_2)_n-\text{O}-\text{CH}_2-\text{CH}_2-\text{OH}$	134-486	2.2-5.6
H	$\text{CH}_2=\text{CH}-(\text{O}-\text{CH}_2-\text{CH}_2)_n-\text{O}-\text{CH}_2-\text{CH}_2-\text{OH}$	132-440	
I	$\text{CH}_3-\text{CH}_2-(\text{O}-\text{CH}_2-\text{CH}_2)_n-\text{O}-\text{CH}_2-\text{CH}_3$	108-558	1.3-2.2
J	$\text{CH}_2=\text{CH}-(\text{O}-\text{CH}_2-\text{CH}_2)_n-\text{O}-\text{CH}_2-\text{CH}_3$	106-384	
K	$\text{OHC}-\text{CH}_2-(\text{O}-\text{CH}_2-\text{CH}_2)_n-\text{O}-\text{CH}_3$	108-382	
L	$\text{OHC}-\text{CH}_2-(\text{O}-\text{CH}_2-\text{CH}_2)_n-\text{O}-\text{CH}_2-\text{CH}_3$	132-528	0.5-0.7
M	$\text{CH}_2=\text{CH}-(\text{O}-\text{CH}_2-\text{CH}_2)_n-\text{O}-\text{CH}=\text{CH}_2$	104-378	
N	$\text{OHC}-\text{CH}_2-(\text{O}-\text{CH}_2-\text{CH}_2)_n-\text{O}-\text{CH}=\text{CH}_2$	130-394	
O	$\text{OHC}-\text{CH}_2-(\text{O}-\text{CH}_2-\text{CH}_2)_n-\text{O}-\text{CH}_2-\text{CHO}$	146-410	

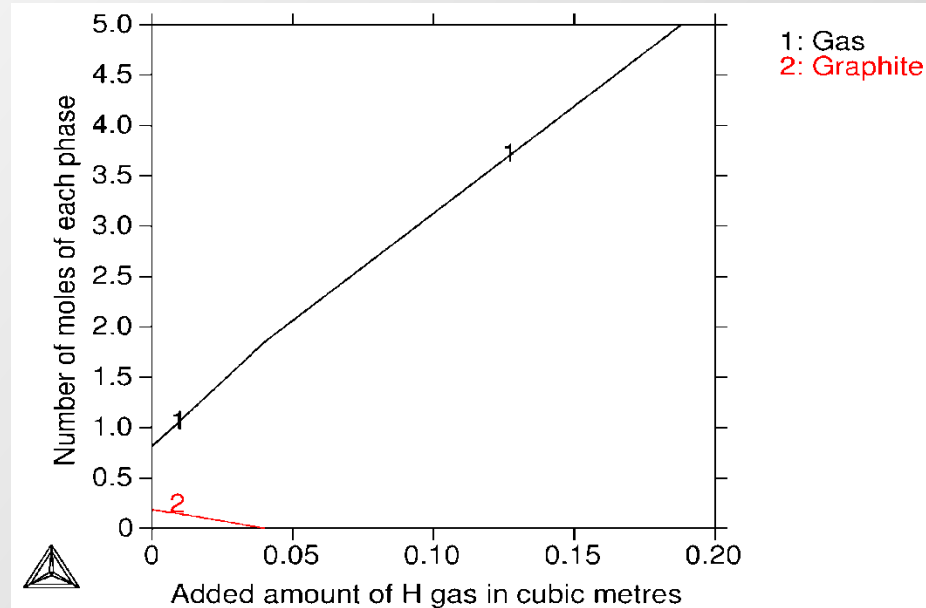
# Modeling debinding in cemented carbides



Large amount of H<sub>2</sub> gas needed to avoid condensation of graphite!

What do we form instead?

T=300°C, H<sub>2</sub>-rich atmosphere,  
Thermo-Calc + SSUB3 database



# Mostly methane and water.

