Models to predict steel microstructure and properties from continuous casting to hot rolling (project ELEMET-Mocastro)

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Project partners in ELEMET- Mocastro

- Ruukki Metals Oy, Raahe
- Outokumpu Stainless Oy, Tornio
- Aalto University
  - Metallurgy (Prof. S. Louhenkilpi)
  - Heat Treatment (Prof. S. Kivivuori)
  - Biomedical Engineering and Computational Science (Prof. J. Lampinen) (statistical algorithms)
- Oulu University
  - Mechanical Engineering (Prof. P. Karjalainen, Prof. D. Porter)
  - Subcontracting; Dept. of Mathematics (fast numerical algorithms)
How do we define the microstructure?

There are many “microstructure scales” in metals and related properties...

We work in this project:

- Nano-scale: inclusions, precipitates
- Micro-scale: dendrites, phases, microsegregations
- Meso-scale: grains, grain growth, homogenisation
- Process scale: heat transfer, as-cast structure
- Related properties

Fig. Courtesy to Prof. Nikolas Provatas, McGill, Canada.
There are also many modelling concepts for different scales. Examples:

MD, PF, CA: need a lot of calculation time and they are not yet very realistic today for multiphase cases with many alloying elements. Also multi-scale and multi-physical modeling is difficult.

Our concept: Fast multi-scale, multi-physical modelling using FDM process models coupled with fast thermodynamic-kinetic-empirical modules. Aim is also on-line use. We do not use MD, PF, CA.
Our aim and motivation

- **Motivation** comes from industry: Higher quality steels are needed all the time. Development and production of new steels are very challenging.

- **Aims**: To develop new multi-scale, multi-physical computer tools to help solving the problems.

**Practical aims:**
1) To develop computationally fast microstructure and property models/tools from continuous casting to hot rolling
2) Coupling of them with the process models
3) On-line applications
4) All models for wide range of steels. So we need new thermodynamic assessment work
Developed models: 1) IDS tool

1. IDS is solidification, microstructure and property model with many modules
2. It is from nano-scale to process scale and also multi-physical
3. We can follow the microstructure evolution from continuous casting to hot rolling, i.e. during solidification, cooling, reheating, holding, rapid cooling
4. Large in-house thermodynamic databank: a lot of new assessment work done for wide range of steels

Fig. Grain boundary concentration and amount of precipitates from CC to hot rolling. Important physical phenomena are among other things homogenisation and dissolution.
**IDS tool**

**INPUT**
- Steel composition
- Cooling rates

**OUTPUT**
- Solidification phenomena
- Phase transformations
- Microsegregation
- Microstructure evolution
- Inclusions
- Precipitates
- Pore formation, etc.

- Thermophysical material properties (H, k, C_p, L,..)
- Thermal contraction
- Density
- Liquid viscosity
- Liquid/air surface tension
- Solid/liquid interface energy
- Hardness, etc.

**Alloying elements included:** Fe, C, Si, Mn, P, S, Cr, Mo, Ni, Nb, Ti, V, B, Al, Ca, Cu, N, O, H. (note: not all elements for all modules)

**Phases:** α-ferrite, Δ-ferrite, eutectic ferrite, austenite, cementite, pearlite, bainite, α-martensite (bct structure), ε-martensite (hcp structure)

**Inclusions/precipitates:** Stoichiometric binaries: AlN, BN, B_2O_3(l), CaO, CaS, CO(g), H_2O(g), MgO, N_2(g), SiO_2, TiB_2, TiO_2, Ti_2O_3, VO; stoichiometric ternaries: Fe_26Al_9C_5, FeMo_2B_2, FeNbB, Fe_2Mo_3O_8, Fe_4Nb_2O_9, Ti_2CS; semi-stoichiometric ternaries: (Mn,Fe)S, (Mn,Cr)S, (C,N)Nb, (C,N)Ti, (C,N)V, (Cr,Fe)_2B, (Ni,Fe)_3B, (Nb,Fe)O_2, (Fe,X)_2B (X=Cr,Mn,Ni,V), (Fe,X)_3O_4 (X=Al,Fe,Mo,V), (Fe,X)_2O_3 (X=Al,Cr,V), (Fe,X)_{0.947}O (X=Cr,Mn,V). **For more complex:** IDS coupled with ChemApp. ChemApp developed by GTT Technologies, Germany.
IDS case: austenite grain growth

It is important to control the grain size during production! → small grain → improved mechanical properties

Grain size depends:
- time
- temperature
- formation of ferrite and precipitates → activation energy, $Q$, increases
- composition

Figure: effect of cooling rate and precipitates:
- Higher cooling → smaller grains
- More precipitates (here Nb(C,N)) → smaller grains
IDS case: calculation of precipitates

It is also very important to control the formation of precipitates for control of grain size, mechanical properties, defects,…

- For calculations, we need equilibrium Gibbs energy ($\Delta G_{\text{MeX}}$) but also nucleation and misfit energies,…
- …coupled with phase transformation and diffusion equations!
- IDS makes that!

Figure:
- Too much precipitates are forming if just $\Delta G_{\text{MeX}}$ is used in the model even if diffusion is included (="strong growth")
- All included = "weak growth"
IDS case example: the effect of cooling rate on precipitation

Many parameters effect on precipitation, one is cooling rate. See the figures below. Same steel composition with different cooling rates. Cooling rate effects on grain growth and diffusion and so on precipitation.

Calculated fractions of Nb(C,N) and AlN in a low alloyed steel cooled with a constant rate of 1°C/s.

Calculated fractions of Nb(C,N) and AlN in a low-alloyed steel cooled with a rate of 10°C/s above 900°C and a rate of 0.05°C/s below 900°C.
Developed process models: 2) continuous casting tool, 3) slab tracking tool after CC to hot rolling

**Continuous casting tool:**
Solidification and heat transfer, fast numerical solution, 3D, possibility for on-line applications

**Slab tracking tool:**
Cooling and heating, fast numerical solution, 3D, tracks each slab after CC, possibility for on-line applications. Also piles included.
Developed models: 4) coupling of IDS with the process models

Cooling rates comes from process models → IDS predicts microstructure evolution. For quality prediction, microstructure control, hydrogen removal from slabs, etc.

**Case 1: Hydrogen removal in the ”H-furnace”**

- IDS calculates H diffusion coefficient ($D_H$) for the steel
- Process model temperature and hydrogen removal from slab. Trapping effect included.

![DH](image)

**Ideal furnace temperature**

*Figure: from $D_H$ we can also see the ideal furnace temperature for each steel grade*

*Case: solidification → cooling → heating → holding → rapid cooling.*

*Ti(C,N) (red curve) and (Fe,Mn)S (blue curve) in a steel cooled with 1°C/s, heated with 1°C/s, hold at 1400°C by 120min and cooled with 10°C/s.*
Main conclusions

- Advanced microstructure and process models have been developed for industrial use from continuous casting to hot rolling.
- It is difficult to study and control complex multi-scale and multi-physical phenomena without advanced computer tools.
- The models are now under validation tests at Ruukki Metals and Outokumpu Stainless.
- Next: on-line applications; more chemical elements into the models, mechanical properties, publications,...
Thank You

Mocastro project