Using XRD in the hunt for cost and CO_2 reduction in the metal and mining industry

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Agenda

- Examples of how modern XRD analysis can provide crucial information in the fight against global warming
  - Iron ore mining and processing
  - Ferrochrome and stainless steel manufacturing and processing

Driving force

Global warming has forced the world to look for solutions to reduce CO_2 emissions:

- New governmental regulations
  - Extra costs and penalties for every unit of CO_2 released into the atmosphere
- New consumer behaviour
  - Important for producers to be at the forefront

Role of XRD

- Efficient tool for identifying the means to reduce CO2 emissions through knowledge of phase composition of starter materials
- Helps in selection of materials that process more efficiently into finished products

Examples from industry

- Iron ore mining
  - Distinguishing between hematite and magnetite is essential for refining the ore and amount of coke needed in the blast furnace
- Production control of ferrochrome and stainless steel
  - Phase analysis of slag is used to optimize conditions and energy consumption during the smelting process

Iron ore

- 650 million tonnes of CO2 per year is emitted from the iron and steelmaking industry
- The reduction step in the blast furnace is the most energy-intensive. Careful control of the phases in the blast furnace is necessary to minimize energy consumption

XRD in the steel industry

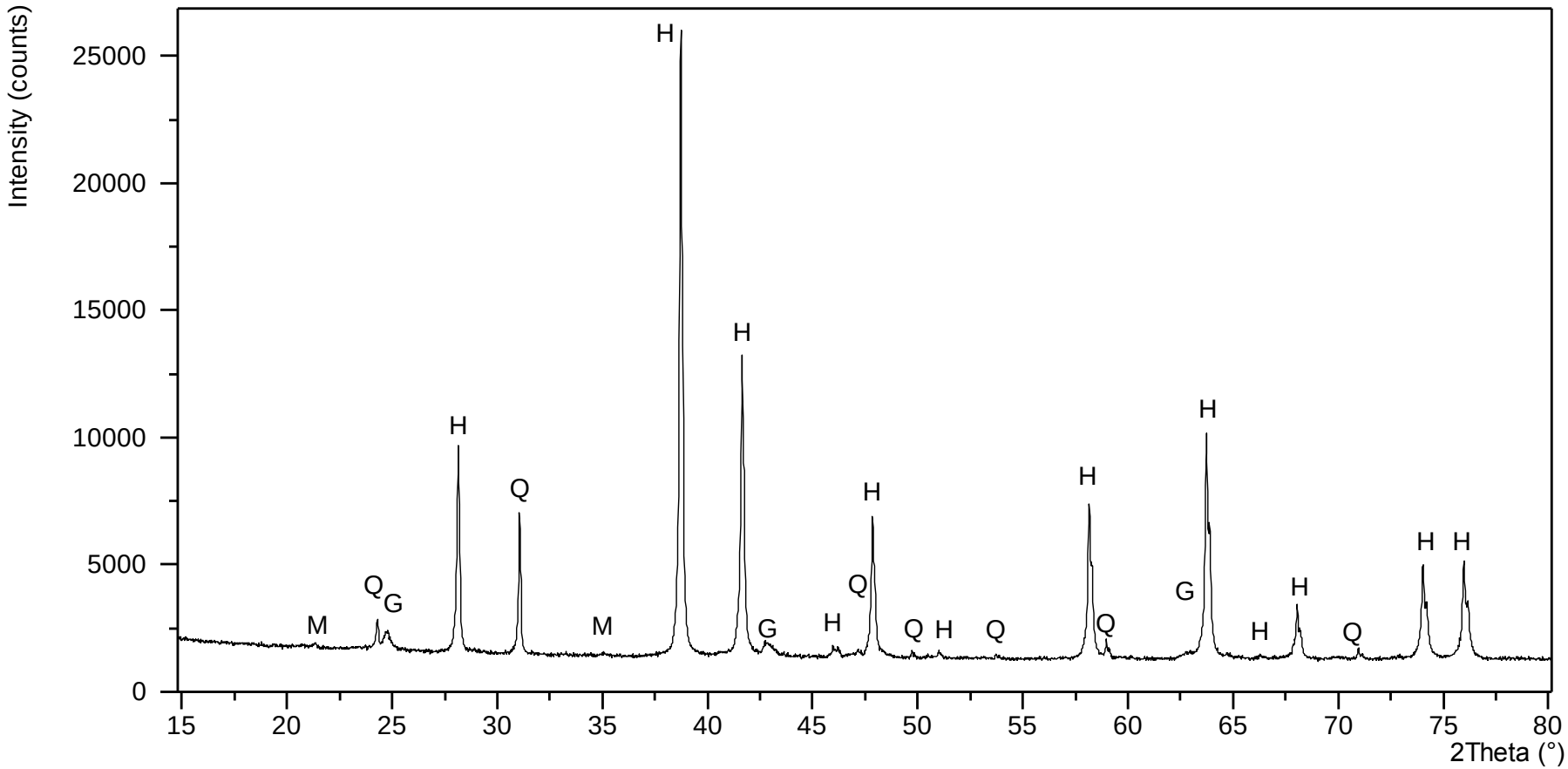
- Many applications:
  - Blending of iron ores
  - Control of the sintering behaviour
  - Quality control of directly reduced iron
  - Analysis of converter slag

XRD methods

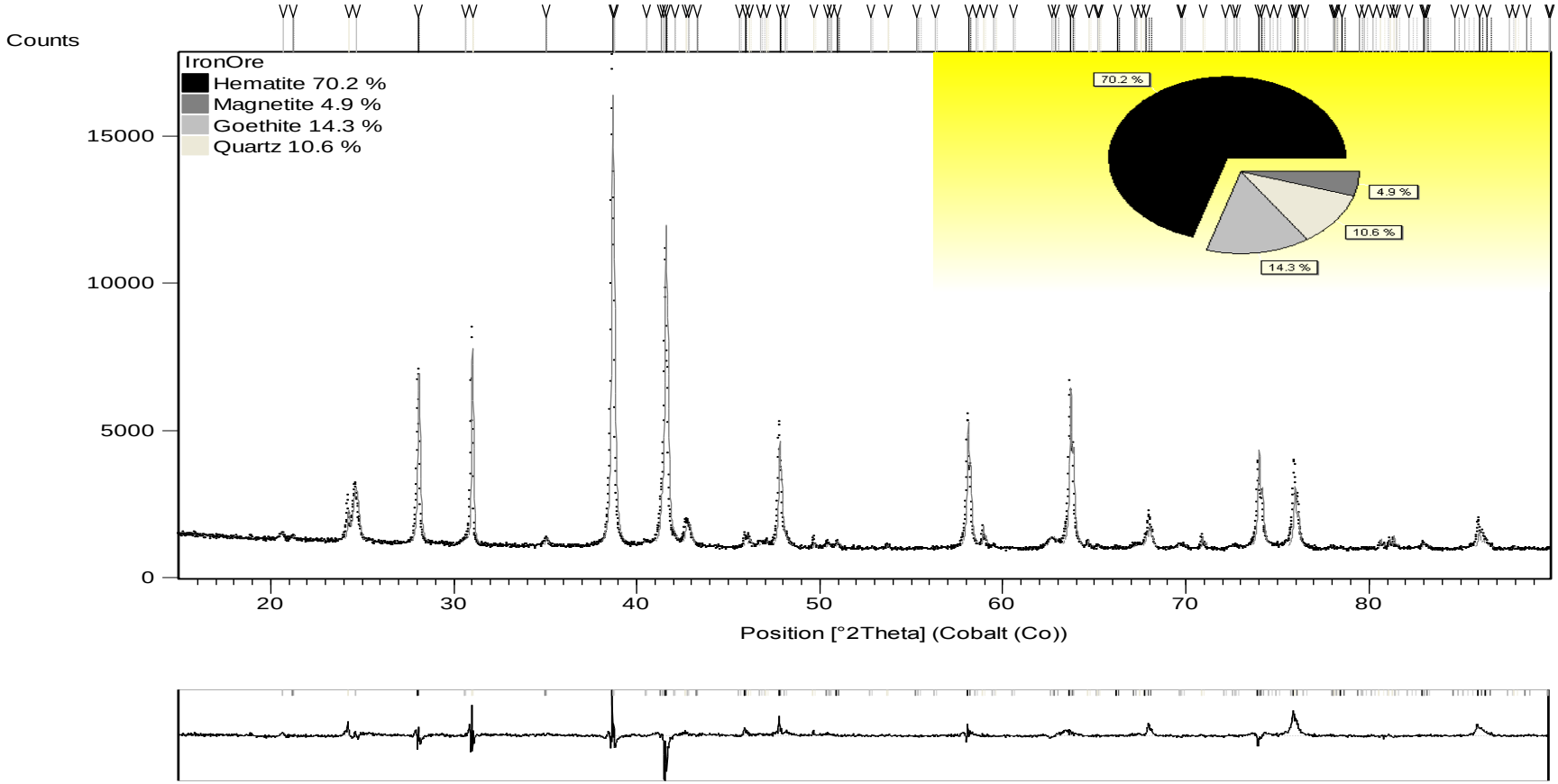
- Traditionally mostly qualitative methods were used
- Faster detectors and the Rietveld method make quantitative analysis possible in less than ten minutes

Measurement and phase identification (iron ore from Brazil)

H=Hematite(Fe_2O_3) M=Magnetite(Fe_3O_4) G=Goethite(FeOOH) Q=Quartz(SiO_2)



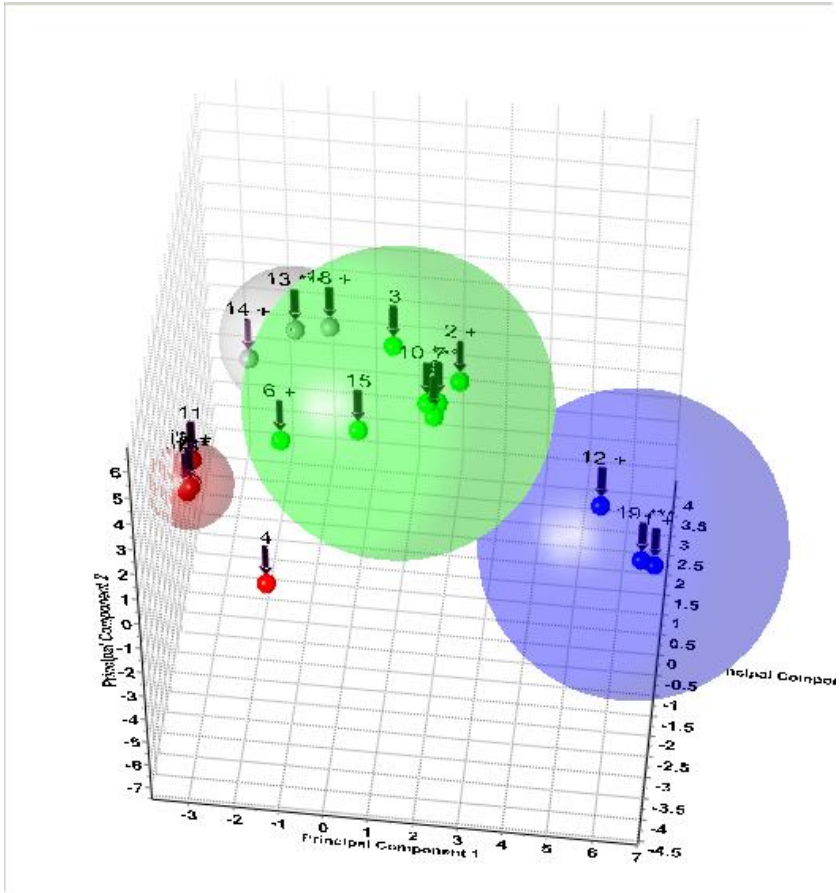
Rietveld refinement results (70% H, 15% G, 5% M, 10% Q)



Cluster analysis – a useful tool

- Statistical method simplifies analysis by
  - Automatically sorting scans into classes of closely related scans
  - Identifying the most representative scan of each class
  - Identifying the two scans of each class that differs the most
  - Identifying outliers not fitting into any class

Cluster analysis: PCA score plot (20 samples)



- Green cluster: high M, medium H, high G, low Q
- Red cluster: low M, high H, low G, low Q
- Blue cluster: high M, low H, high G, high Q
- Grey cluster: low M, high H, low G, high Q
- Larger sphere = more variation within the group

Ferrochrome and stainless steel

- 90% of mined chromite is converted into different grades of ferrochrome
- 80% of ferrochrome is used in stainless steel
- This example comes from Outokumpu where recycled steel is used as raw material
- Reduces CO_2 emissions drastically but makes control of raw material even more important

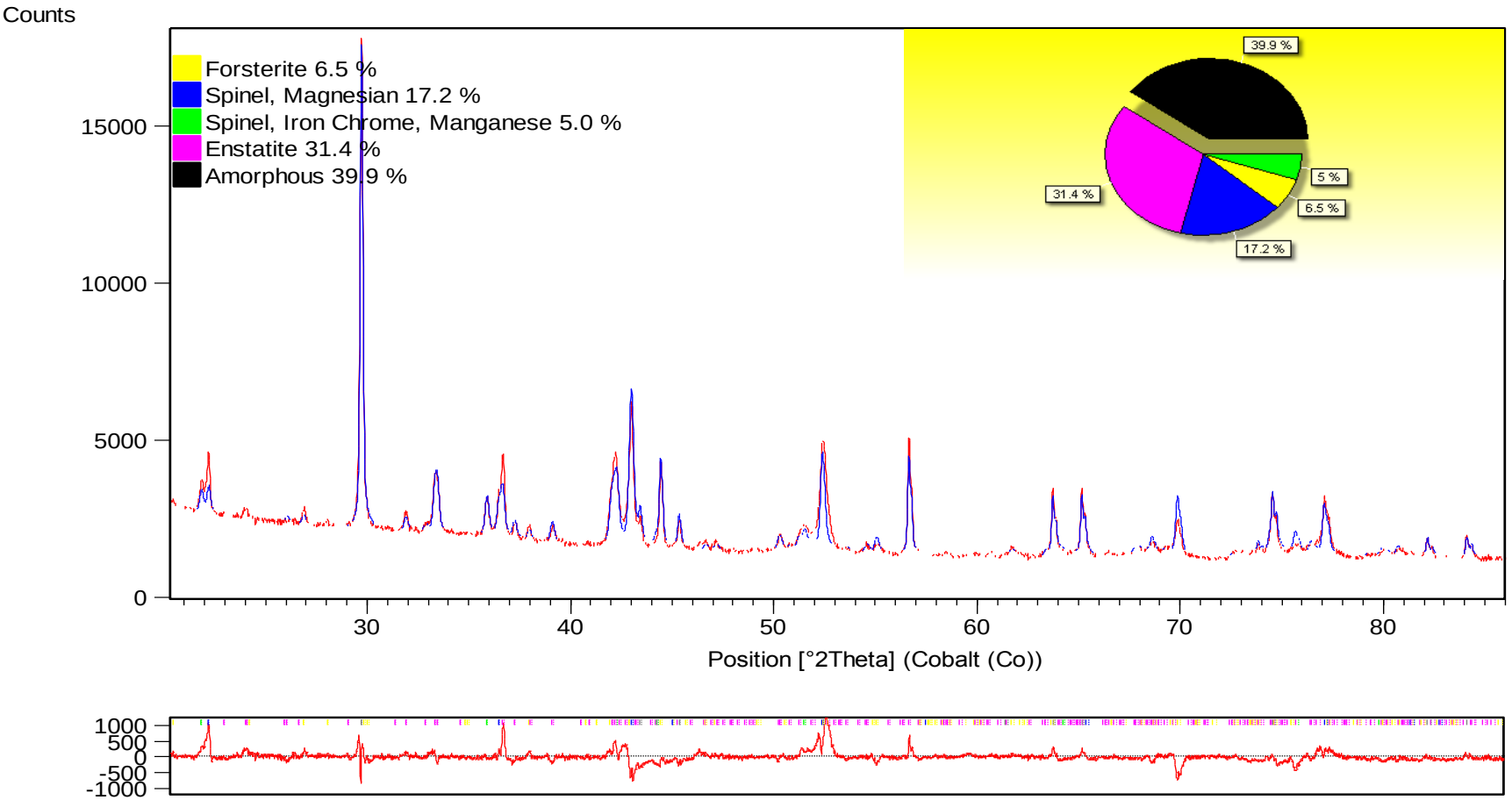
Use of XRD

- Monitor the composition of different slag materials to control steel making process
- Phase composition of slag reflects
  - Material and energy efficiency of the furnace
  - Presence of impurities
  - Lifetime of refractories
- Slag can be used as road fill, in building materials, ballast, …

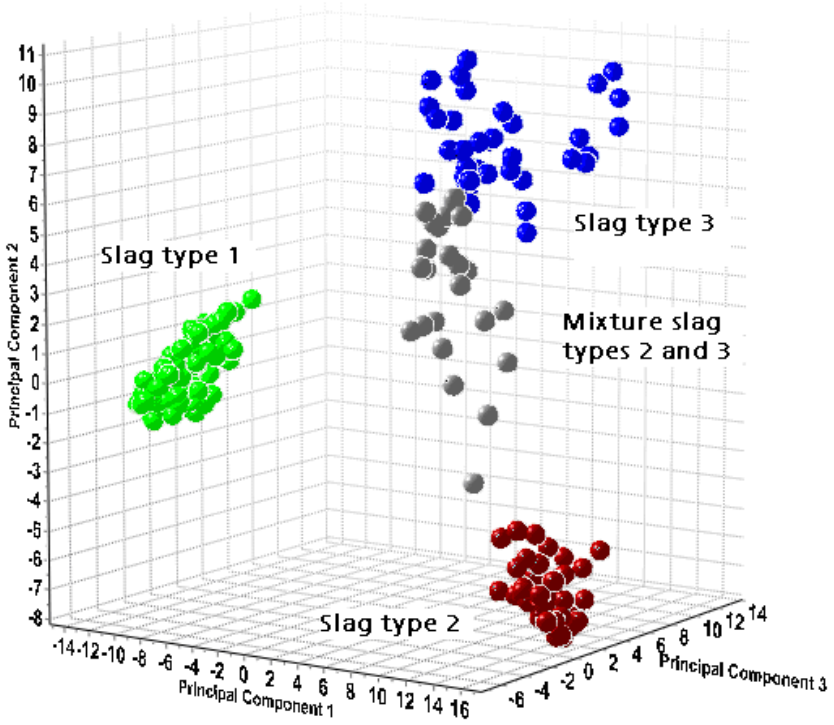
Slag types identified

Slag Type 1	Slag Type 2	Slag Type 3
Forsterite Mg_2SiO_4	Merwinite $Ca_3Mg(SiO_4)_2$	Bredigite $Ca_7Mg(SiO_4)_4$
Spinel $MgAl_2O_4$	Melilite $(Ca,Na)_2(Al,Mg,Fe)(Si,Al)_2O_7$	Fluorite CaF_2
Spinel $(Mg,Fe)(Al,Cr,Fe)_2O_4$	Periclase MgO	Larnite Ca_2SiO_4
Enstatite $MgSiO_3$	Calcite $CaCO_3$	Periclase MgO
amorphous part	Monticellite $CaMgSiO_4$ + amorphous part	amorphous part

Rietveld refinement for a slag type 1



Cluster analysis: PCA score plot 220 slag samples



- 4 different clusters of scans have been identified

Information from phase analysis

- Different phases found are used as monitors for certain steps in the process
  - Fe-Cr-spinel: temperature and energy consumption
  - Crystalline/amorphous ratio: cooling conditions

Conclusions

- XRD provides valuable information for mining and process control in the mining industry through standardless quantification and fast, statistical evaluation of large sets of data through cluster analysis
- Modern optics, detectors and software provide accurate analyses within minutes