Diffusion data need for Heat Treating Industries

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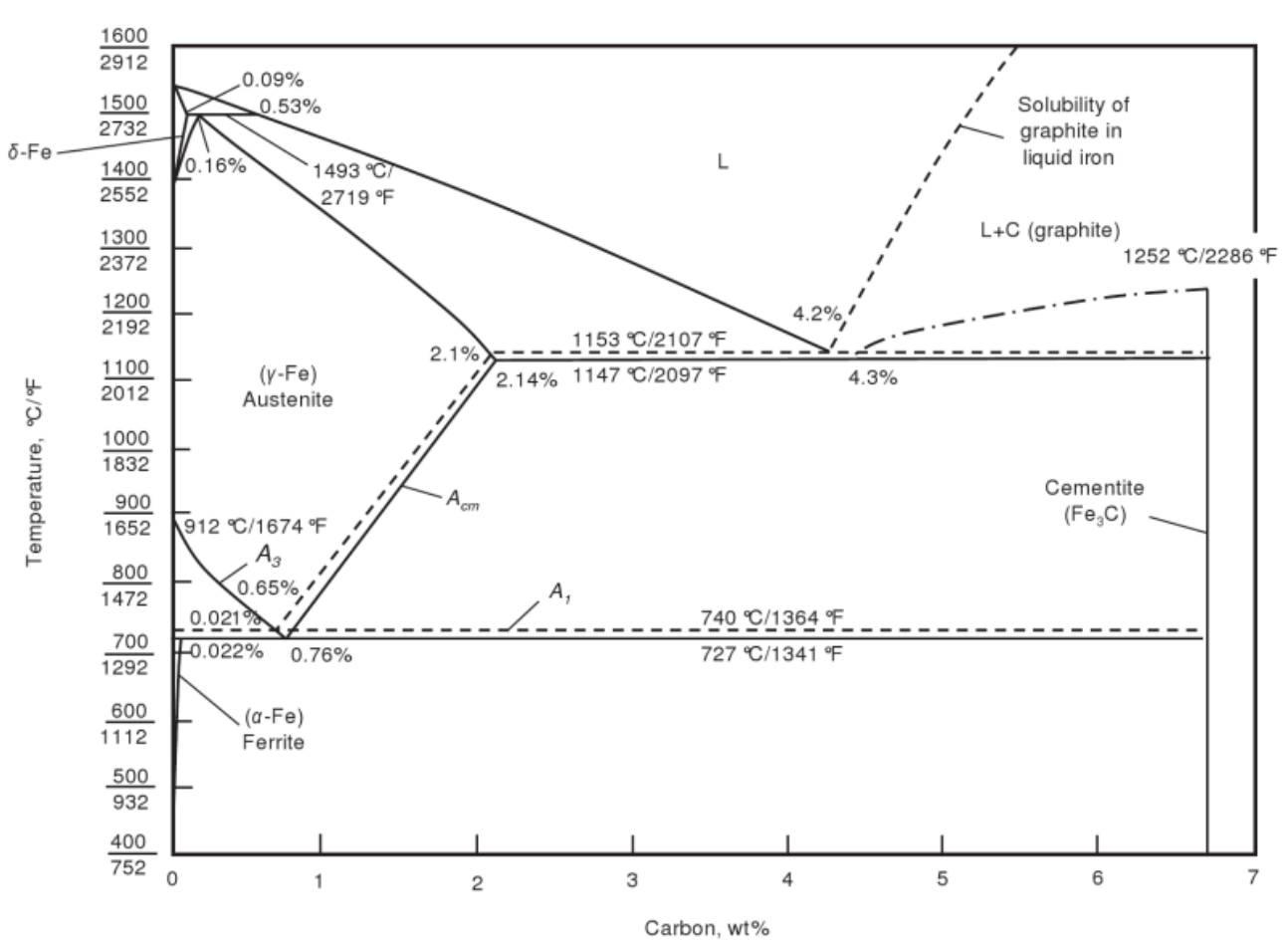
Heat treatment processes

- Direct Hardening
- Surface Hardening

Tools used by the heat-treaters

Phase diagram



Solid lines indicate Fe-Fe_3C diagram; dashed lines indicate iron-graphite diagram.

Fig. 10.1 The Fe-Fe_3C diagram. Source: Ref 1

Source: Flake C. Campbell, Elements of Metallurgy and Engineering Alloys, ASM International, Jun 30, 2008

Isothermal transformation diagram

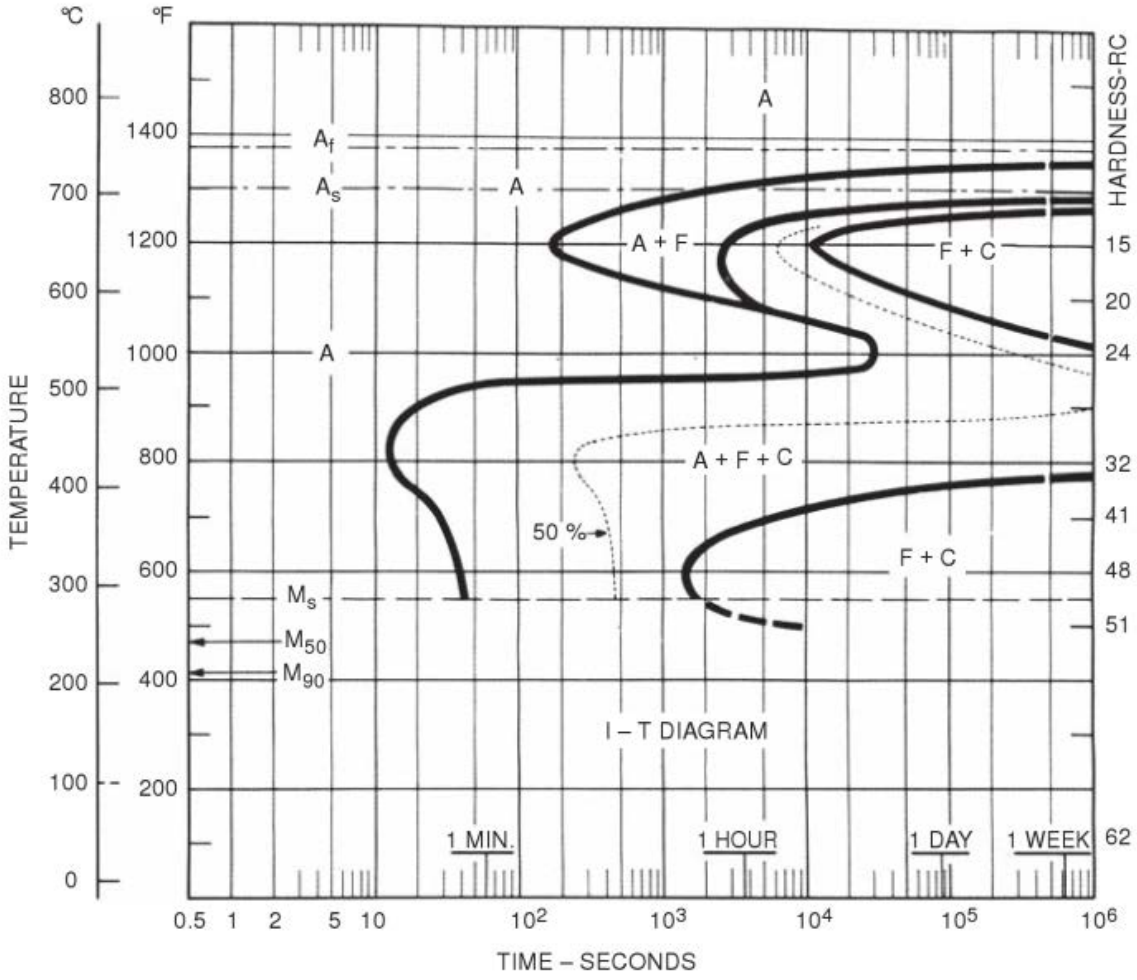


Fig. 11.8 Isothermal transformation diagram for 4340 steel. Austenitized at 870 °C (1600 °F), ASTM grain size 6–7. Source: Ref 4

Source: Flake C. Campbell, Elements of Metallurgy and Engineering Alloys, ASM International, Jun 30, 2008

Continuous cooling transformation diagram

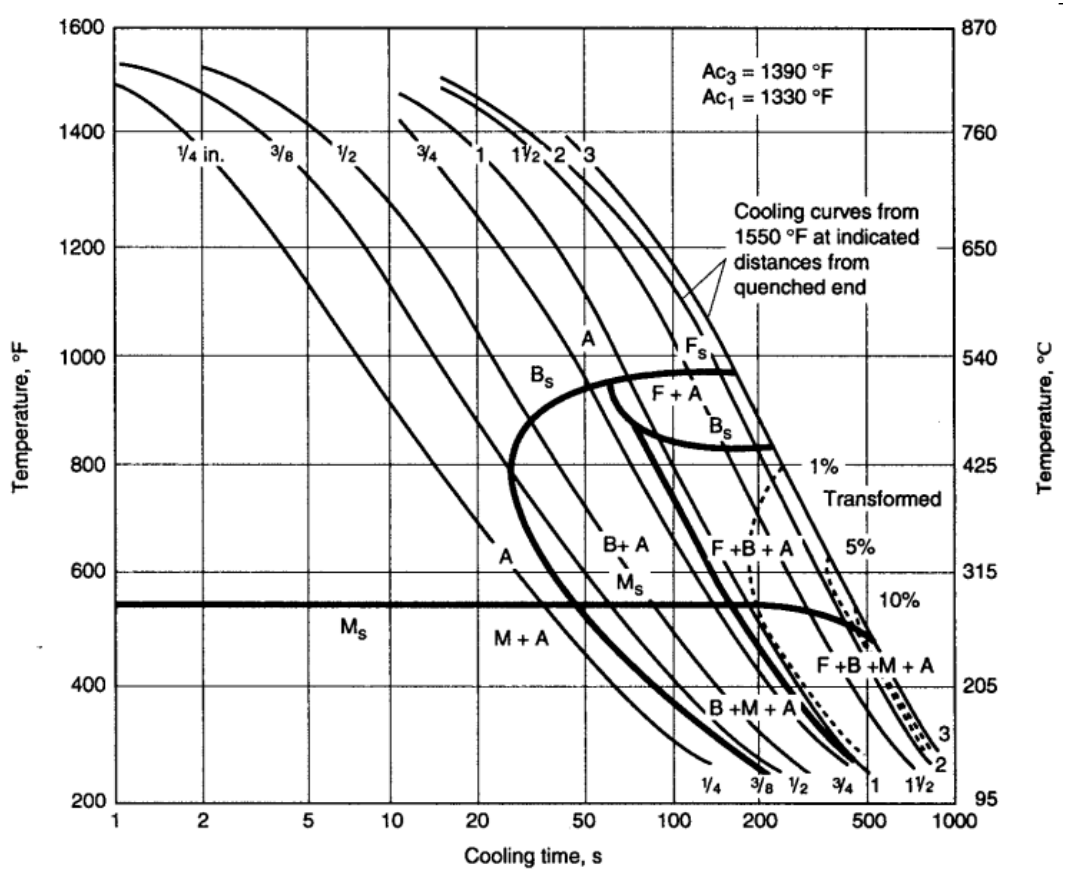


Fig. 11.9 Continuous cooling transformation diagram for 4340 steel. Source: Ref 5

Source: Flake C. Campbell, Elements of Metallurgy and Engineering Alloys, ASM International, Jun 30, 2008

Heat treating industry needs

Needs

- Better prediction and model of
  - the phases present in steels,
  - the microstructures of steel
  - the resulting physical properties of steel during and after processing.

  - Addressing these questions has many practical implications
    - not just for the usage of the final product,
    - but also for the optimizing the production and processing aspects of steels.
    - Increased predictive capabilities through ab initio modeling can thus be anticipated to have significant practical benefits.

- For a multi-component alloy system
  - Thermodynamics
  - Precipitation kinetics
  - Diffusion
  - Phase transformation
  - Microstructure

Simulation scenario

- Casting and solutionizing
- Casting, heat treatment and welding
- Precipitation kinetics in micro-alloyed steel
- Carburization, quench and temper

Simulation software

- Easy to use
- Pre- and post-processing through GUI-based
- Scripting capabilities in the back-end
- Universal interface for exporting data
  - Coupling with macroscale modeling software (FE/FD) for property/microstructure prediction

Casting

- Microsegretation of alloying elements
- Gas porosity prediction

Precipitation kinetics

- Precipitate/matrix volumetric misfit
- Temperature dependent Young's modulus,
- Composition-, temperature- and size-dependent interfacial energies,
- Bulk and grain boundary diffusion

Tempering kinetics

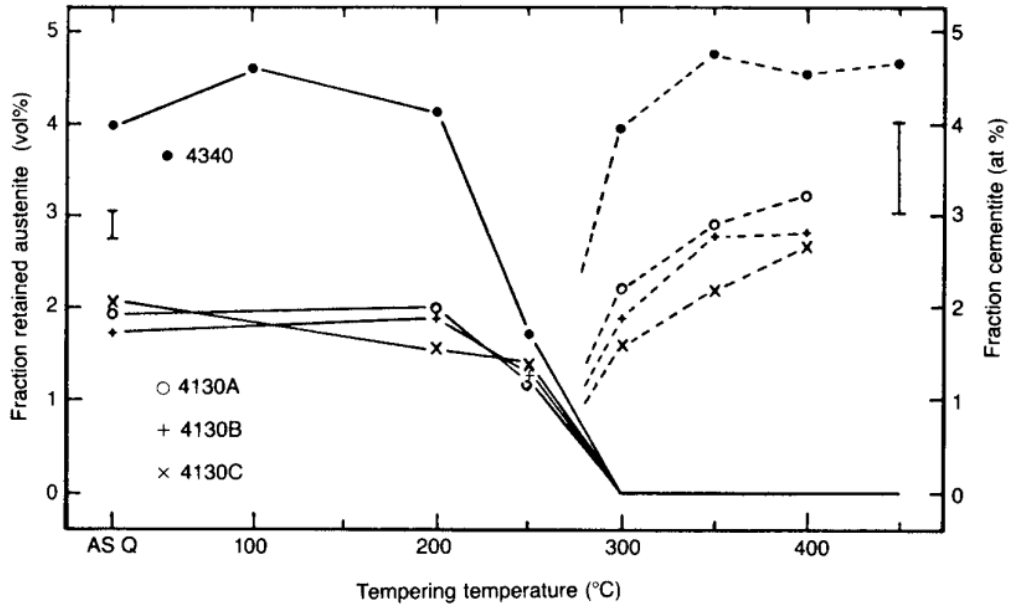


Fig. 11.23 Transformation of retained austenite in 4130 and 4340 steels. Source: Ref 10

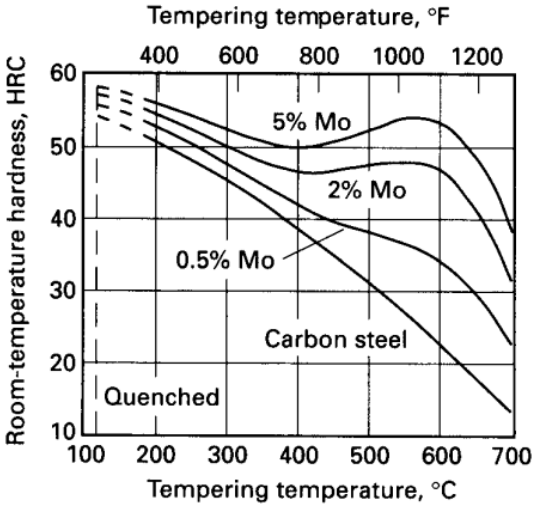


Fig. 11.24 Secondary hardening of molybdenum alloy steels. Source: Ref 11

Source: Flake C. Campbell, Elements of Metallurgy and Engineering Alloys, ASM International, Jun 30, 2008

Martensitic transformation

- Modeling athermal transformation
  - Predicting retained austenite fraction
- Temper kinetics of martensite