Models for the Yield Strength of Al-Zn-Mg-Cu Alloys

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Introduction

- Al-Zn-Mg-Cu alloys are important in structural applications, esp. where high specific strength is required.
- Al-Zn-Mg-Cu alloys are mainly used in overaged condition

Aims:

Construct a model for the yield strength of overaged Al-Zn-Mg-Cu alloys that includes:

- Microstructure development / precipitation / coarsening
- Solution strengthening (Zn,Cu,Mg)
- Precipitation strengthening
- Computationally simple description of influence of Mg/Zn/Cu on strength
- Both for Zr or Cr grain refiner additions

➢ Part of continuing effort on modelling of properties of a range of heat treatable Al based alloys.

Contents

- Model structure
- Model details
- Modelling results
- Verification of the model
- Conclusions

Previous work

- Some recent work on evolution of precipitates uses Kampman-Wagner type iterative procedures

$$\frac{dr}{dt} = \frac{\overline{X} - X_i(r)}{X_p - X_i(r)} \frac{D}{r}$$

- allows calculation of evolution of precipitate size distribution evolution on rapid heating
- at present only applied for spherical precipitates

A. Deschamps and Y. Brechet, *Acta Mater. 47, 1998*

M. Nicolas, A. Deschamps, *Acta Mater, 2003*

- Strengthening due to plates and rods has been analysed

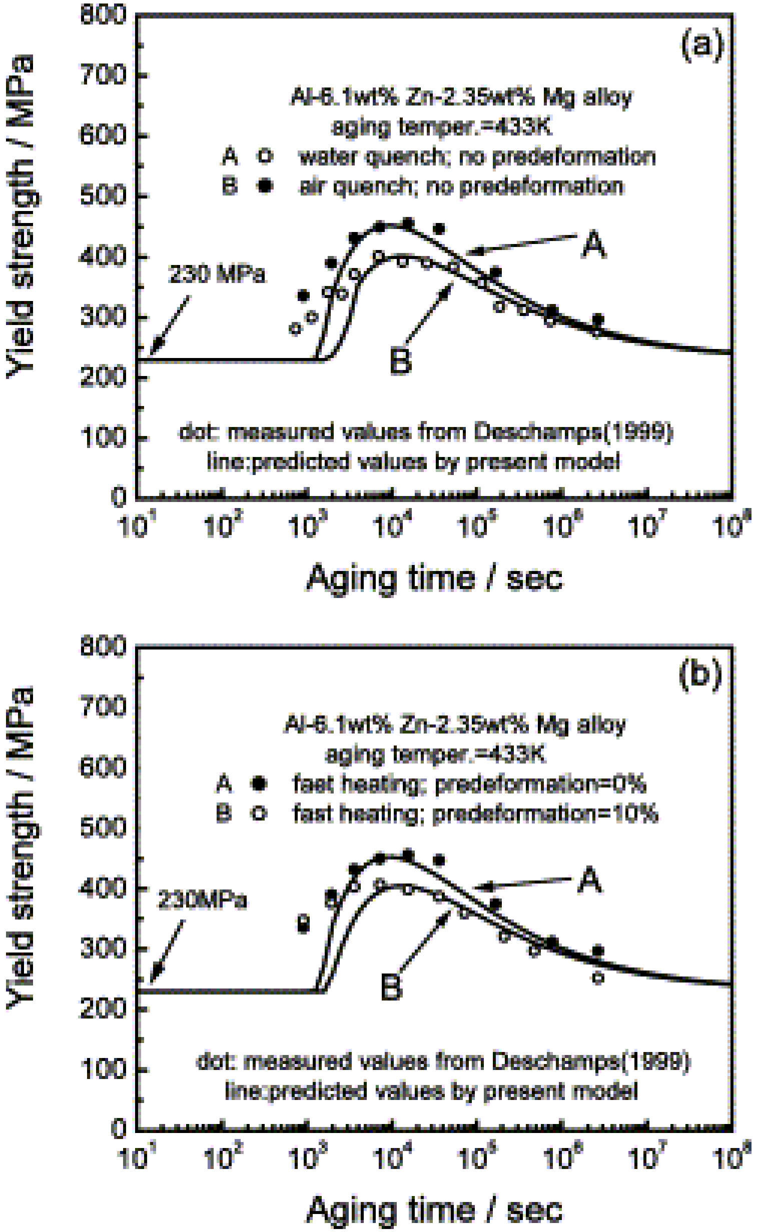
  e.g. for plates lying parallel to {111} planes

$$\Delta\tau_{prec} = 0.12G\frac{b}{(l_D l_t)^{1/2}}\times\ln\frac{0.079l_D}{r_{cut}}\times\left[f^{1/2}+0.70\left(\frac{l_D}{l_t}\right)^{1/2}f+0.12\left(\frac{l_D}{l_t}\right)f^{3/2}\right]$$

[Zhu, Starke, *Acta Mater 344, 1999*]

- Incorporated in strengthening models for Al-Zn-Mg alloys

Liu, Zhang, Ding, Sun, Chen, *Mater Sci Eng A, 344, 2003*



Model structure

Microstructure development: precipitation / coarsening model

- equilibrium state predicted / approximated using effective solute content
- effectively one strengthening precipitate phase present in overaged condition
- composition of precipitate dependent on alloy composition; but independent of ageing time
- precipitation / coarsening approximated by novel simplified approach encompassing JMAK type and LSW type approaches: no iterative schemes

Microstructure-strengthening model

- increments in critical resolved shear strength (CRSS) of grains due to precipitation and solution hardening
- precipitates are non-shearable discs
- texture is included

Calibrating model parameters strength Al-Zn-Mg-Cu

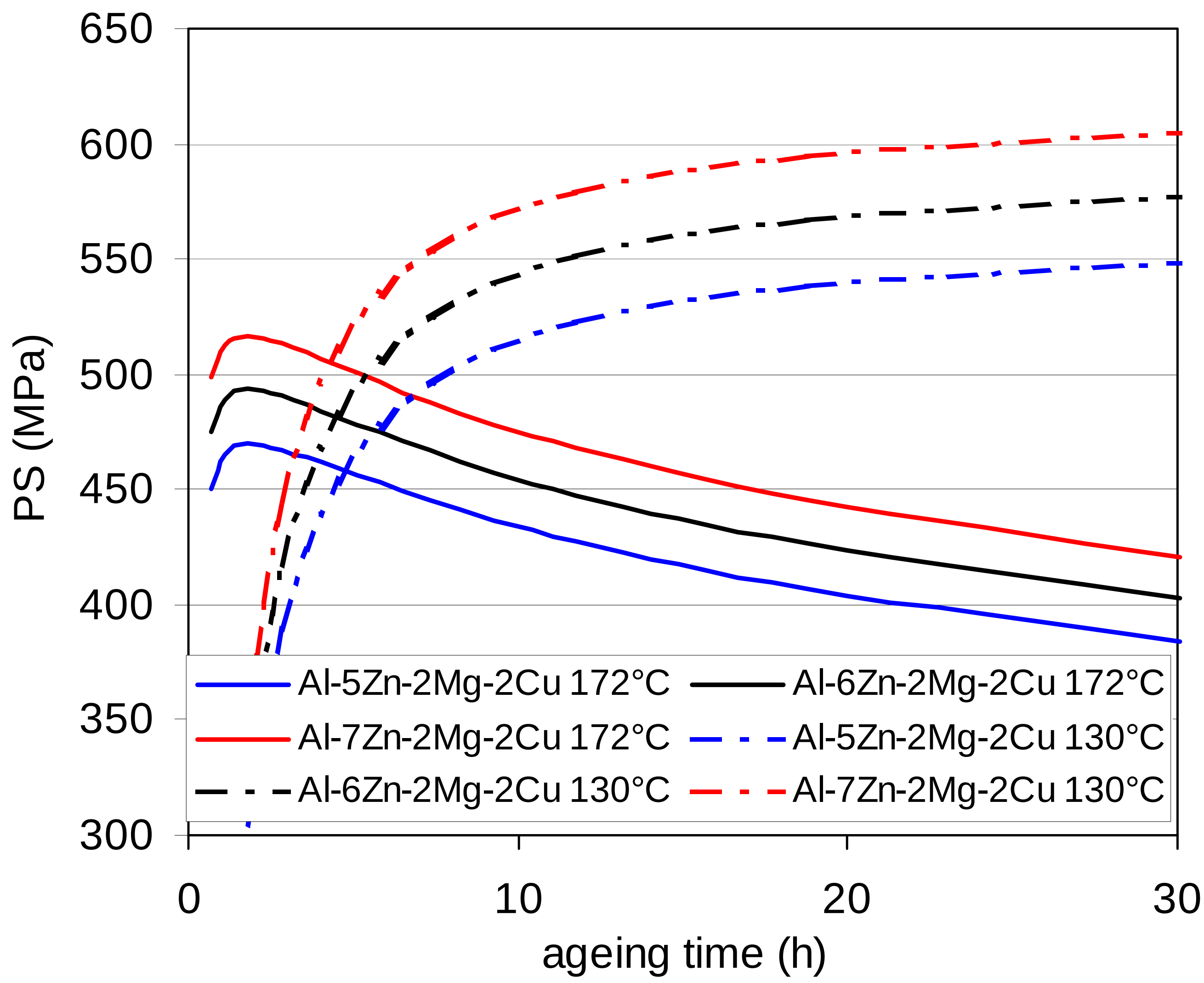
- model contains ~30 equations, ~30 parameters

  E.g.

  $$\bar{l}_c^{\,3}(t) - \bar{l}_0^{\,3} = k_c(T)t$$ (LSW coarsening law)

- all parameters are either
  - physical quantities, or
  - related to physical quantities
- most parameters can be determined directly from microstructural analysis or literature data
- parameters that are not accurately known (4) can be calibrated by fitting to the yield strength data
- validation of model is achieved by
  - predicting strength of ‘unseen data’ in a train and test procedure
  - comparing the calibrated parameters with physical understanding
  - comparing predictions on precipitate size with TEM data

Example of model output



The Model: Metastable Equilibrium

- Literature data indicates that composition of strengthening precipitate is closely linked to alloy composition.
- We consider an effective amount of atoms forming a precipitate:

$$c_S = x_A + B_B x_B + B_C x_C + ...etc$$

- And take solvus to be approximated by

$$c_0 = c_S \exp\left[-\frac{Q_S}{R}\left(\frac{1}{T}-\frac{1}{T_{S,R}}\right)\right]$$

The Model: Precipitation Kinetics

- Transformed fraction $\alpha(T,t)$, the amount of precipitate $x(t)$ and the solute concentration $c(t)$:

$$\alpha(T,t) = 1 - \left[\frac{[K(T)t]^n}{\eta_i} + 1 \right]^{-\eta_i}$$

α:	fraction transformed,
η_I:	impingement exponent,
n:	reaction exponent / Avrami exponent
$K(T)$:	rate constant for precipitation, depends on alloy content
$k_c(T,f)$:	rate constant for coarsening
l_0:	initial average size of the precipitate

Average precipitate size:

- The average size of the precipitate in nucleation and growth stages:

$$\bar{l}_g(t) = \bar{l}_o \alpha^{1/3}$$

- The average size of the precipitate in coarsening stage:

$$\bar{l}_c^{\,3}(t) = \bar{l}_0^{\,3} + k_c(T, f)t$$

  - rate constant dependent on volume of precipitates

- The average size throughout the nucleation-growth-coarsening process:

$$\bar{l}(t) = \bar{l}_g(t) + \bar{l}_c(t) - \bar{l}_0$$

The Model: Strengthening Model

- CRSS increment due to solution strengthening: $\Delta\tau_{ss} = C_3 c^{2/3}$

- CRSS increment due to precipitation strengthening by non-shearable discs lying parallel to {111} planes:

$$\Delta\tau_{prec} = 0.12G \frac{b}{(l_D l_t)^{1/2}} \left[f^{1/2} + 0.70 \left(\frac{l_D}{l_t} \right)^{1/2} f + 0.12 \left(\frac{l_D}{l_t} \right) f^{3/2} \right] \ln \frac{0.079 l_D}{r_{cut}}$$

- Superposition of the strengthening:

$$\tau_{tot}(t) = \Delta\tau_0 + \Delta\tau_{ss} + \Delta\tau_{d\&ppt}$$

- Yield strength:

$$\sigma_y = \Delta\sigma_{gb} + M\,\tau_{tot}$$

G:	shear modulus
b:	Burgers vector
c:	solute concentrations in matrix
f:	volume fraction of precipitates
l_d:	diameter of the precipitate
l_t:	thickness of the precipitate
M:	Taylor factor
σ_{gb}:	grain boundary strengthening)

The Model: Texture

- Texture of 13 representative alloys determined using EBSD
- Schmidt factors calculated
- M taken as average M for activation of 3 or 4 slip planes (self consistent model)

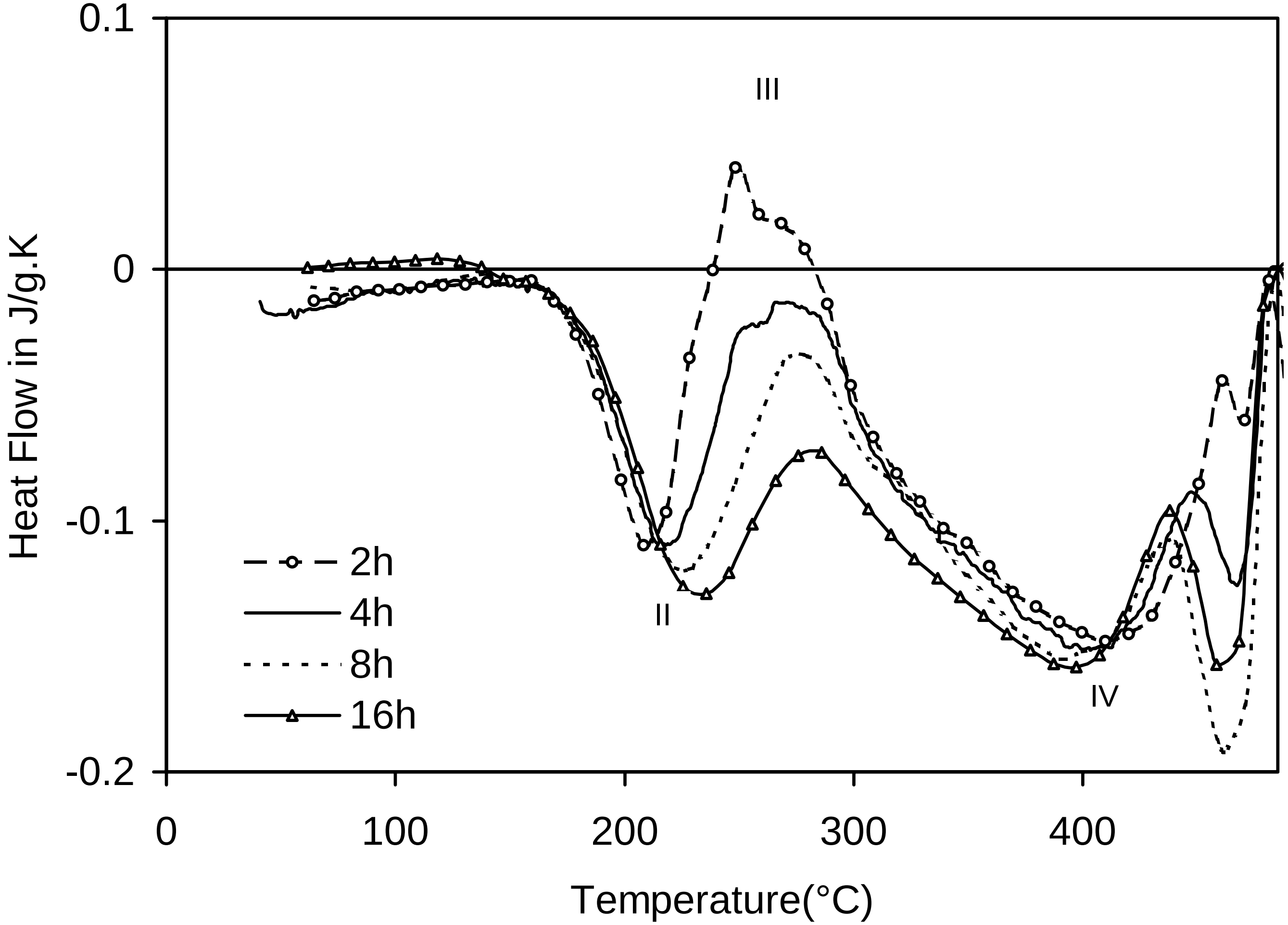
Calibrating model parameters

- Most parameters can be calibrated from microstructural data
- Published 3DAP data -> aspect ratio discs
- Published time to peak hardness data -> k
- Data on extensive overageing 7050 provides solution strengthening factor C_3

Further parameter calibration using database on strength:

- Total 20 Al-Zn-Mg-Cu alloys with compositions spread over main 7xxx alloys 7x50, 7449, 7010, 7x75; tested in rolling direction.
- 15 Zr containing alloys
- 5 Cr containing alloys
- selected alloys studied by DSC, TEM, EBSD

Model calibration: Microstructural Analysis



DSC curves of Al-6.1Zn-2.3Mg-2.6Cu-0.1Zr alloy aged at 172°C

- Ts ≈ 290°C

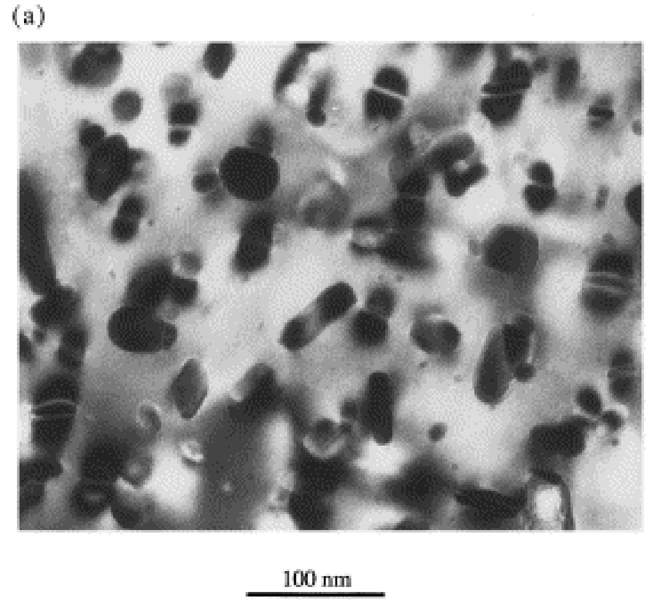
Verification / validation of the model

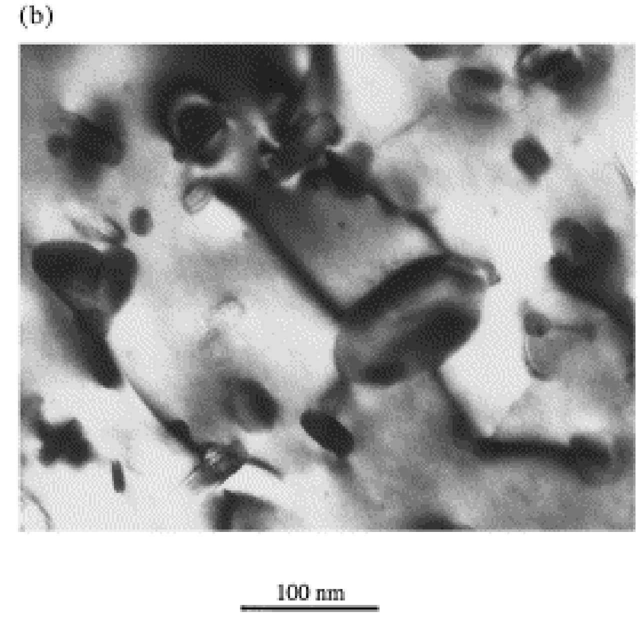
I. Precipitate sizes

literature data available

TEM from

Deschamps, Livet and Bréchet, Acta Materialia, 47, 1998, 281-292





TEM micrographs Al-6.1Zn-2.35Mg-0.1Zr 700 h at 160°C.

(a) Undeformed material

(b) material predeformed 10%.

Predicted vs. measured diameter of precipitates

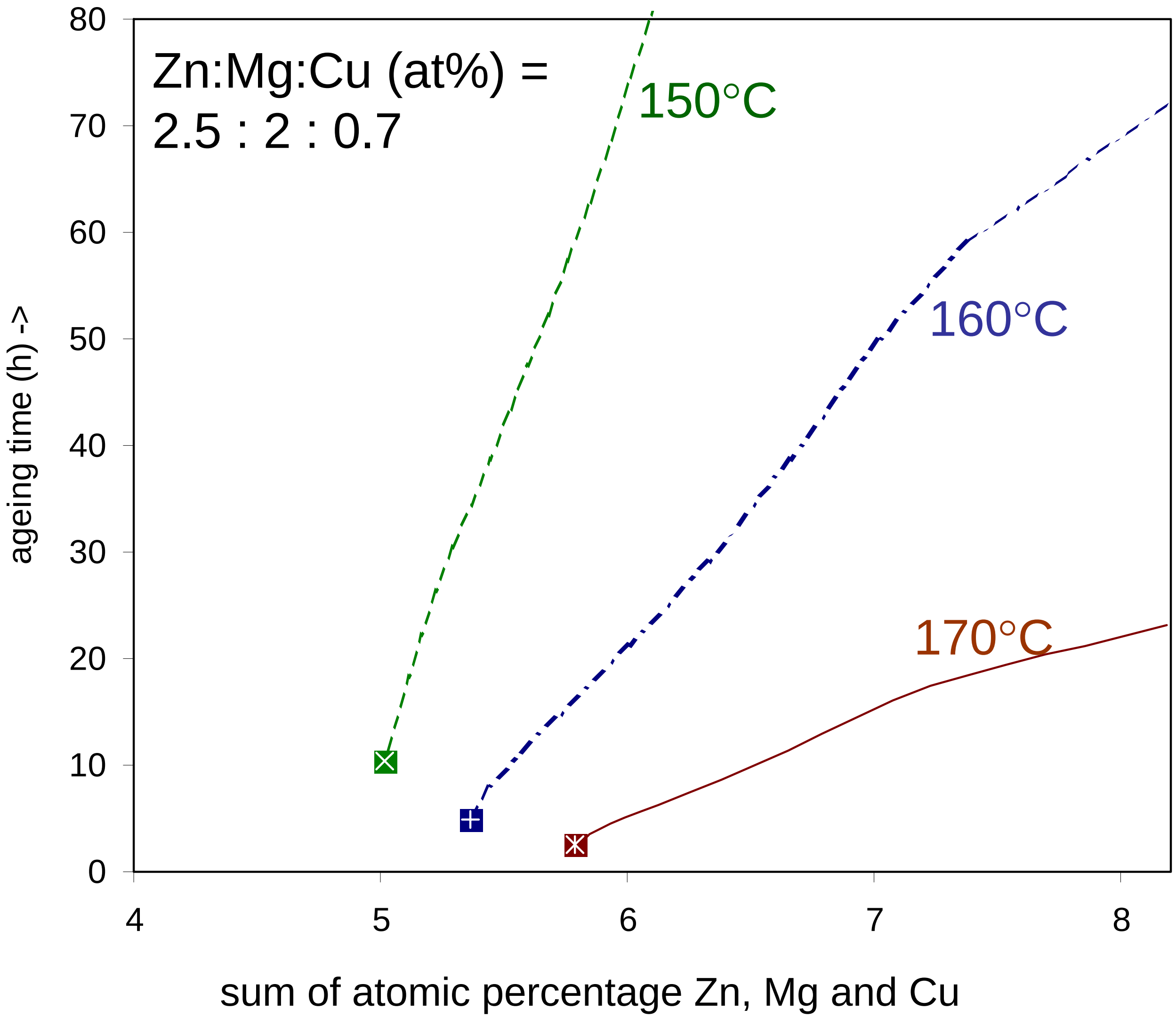
Alloy (wt%)	Ageing treatment	Diameter Measured* (nm)	Diameter Predicted (nm)
Al-6.1Zn-2.35Mg-0.1Zr	50h/160°C	16	21
Al-6.1Zn-2.35Mg-0.1Zr	700h/160°C	52±5	49
Al-5.5Zn-1.2Mg-0.16Zr	7h/170°C	20	14
Al-5.5Zn-1.2Mg-0.16Zr	7h/150°C	11	9
Al-6.1Zn-2.3Mg-2.6Cu-0.1Zr	16h/172°C	19±3	20
Al-6.7Zn-2.9Mg-1.9Cu-0.1Zr	16h/172°C	20±5	20
7475 (~ Al-5.7Zn-2.3Mg-1.6Cu-0.2Cr)	1320h//160°C	59	61

- Predictions correspond well with measured precipitate sizes

* TEM data from:
Deschamps, Livet, Brechet, Acta Mater. 1999; 47: 281
Werenskiold, Deschamps, Bréchet, Mater. Sci. Eng. A 2000; 293: 267
Poole, Shercliff, Castillo, Mater. Sci. Techn. 1997; 13: 897
Li, Starink, Proc of 1st Symp Modeling Al alloys, Pittsburgh, 2003

Model capabilities: inverse predictions

Ageing time required to obtain a yield strength of 500 MPa for alloys with 39% recystallisation.



Conclusions

- Derived / assembled physically based model for predicting yield strength of Al-Zn-Mg-Cu alloys; ~30 equations, ~30 parameters.
- Model characteristics
  - no iterative schemes used
  - influence Zn, Mg, Cu on strength through linear combination
  - strengthening due to disc-shaped non shearable particles with composition depending on alloy composition
  - temperature and composition dependent formation rates of the particles
  - volume fraction dependent coarsening of precipitates
  - solution strengthening
  - texture influence
- Accuracy of model on predicting strength unseen data: 14 MPa
- Verification of model by analysis published data on precipitate sizes in overaged 7xxx alloys

Continuing / future work

- Composition dependency of coarsening rate
- Integrate all published approaches into one model, e.g. Wagner-Kampmann iterative scheme into present model.
- Variation in precipitate shape with ageing

Acknowledgements

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