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Predicting microstructure and strength of maraging steels: Elemental optimisation

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ABSTRACT

A physics-based modelling framework to describe microstructure and mechanical properties in maraging steels is presented. It is based on prescribing the hierarchical structure of the martensitic matrix, including dislocation density, and lath and high-angle grain boundary spacing. The evolution of lath-shaped reverted austenite is described using grain-boundary diffusion laws within a lath unit. The dislocation density provides the preferential nucleation sites for precipitation, whereas descriptions for particle nucleation, growth and coarsening evolution are identified for Ni₃Ti, NiAl and its variants, and BCC–Cu clusters. These results are combined to describe the hardness at different ageing temperatures in several Fe–Ni–, Fe–Mn– and Fe–Ni–Mn–based steels. A critical assessment on individual contributions of typical alloying elements is performed. Ni and Mn control the kinetics of austenite formation, where the latter shows stronger influence on the growth kinetics. Ti additions induce higher hardness by precipitating stronger Ni₃Ti, whereas Cu clusters induce low strength. A relationship between the reverted austenite and the total elongation in overaging conditions is also found. This result allows to identify optimal process and alloy design scenarios to improve the ductility whilst preserving high hardness in commercial maraging steels.

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1. Introduction

Maraging steels combine exceptional properties, including high strength and toughness, high strength to weight ratio, good weldability, simplicity of heat treatments and dimensional stability. These properties stem from the complex microstructures forming during hot processing: (i) A hierarchically-arranged lath martensite matrix (α') decorated by (ii) nano-sized intermetallic precipitates and (iii) austenite laths (γ) that re-precipitate from α' . The first two items dictate mostly the hardness, whilst the partial reversion from martensite to austenite strongly influences their ductility and toughness [1,2]. Additionally, complicated interactions between alloying elements and the evolving microstructure occur during ageing. For instance, grain-boundary embrittlement occurring in underaged conditions is due to Mn and Ni segregation to the prior-austenite boundaries, becoming ductile again during overaging [1,2]. This effect is induced by austenite reversion, promoting Ni and Mn partitioning into the γ , and by overaging

grain-boundary precipitates [1].

Systematic experimental studies have been performed to explore optimal compositions for improving the mechanical properties of maraging steels [3–7], whilst optimisation algorithms have been postulated to link alloying additions with strength variations [8–10]. Although the optimisation methods show good correlation with experiments, no detailed microstructural information is predicted; this limits their application to other compositional scenarios. Additionally, thermokinetics methods have been applied to understand how the chemical composition affects intermetallic [11] and reverted austenite [12,13] evolution; however, these approaches have not provided a direct link with mechanical properties, including strength and elongation.

These results show that, in spite of the considerable work done to improve the properties of maraging steels, a unified physics-based modelling framework is missing. Such could provide direct links between the microstructure and mechanical properties for different compositions and heat treatments. A key reason for this is the lack of a description for the martensitic matrix, as its hierarchical structure strongly controls microstructure evolution [6,12,14]: a high dislocation density in the laths accelerates

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precipitation nucleation, whereas the segregation of γ -stabilising elements into the lath boundaries determines the morphology and kinetics of the reverted austenite [14–16].

The objective of this work is to present a modelling suite for describing microstructure evolution and mechanical properties in maraging steels, including effects of chemical composition and initial microstructure. The models are based on a previous description of the hierarchical structure of lath martensite in Fe–C steels [17,18], where the density of dislocations, laths, and high-angle grain boundaries were prescribed in terms of the prior-austenite grain size and ageing conditions; the extension of the martensite models to maraging steels is presented in Section 3. These features will allow us to provide the microstructural landscape for modelling reverted austenite and precipitation evolution in Sections 4 and 5, respectively. These results are combined in Section 6 to link the resulting microstructure with the hardness of maraging steels. Model validation with experimental data in 19 steels is presented in Sections 7 and 8. A critical assessment on individual contributions of the typical alloying elements to the yield strength and ductility is presented in Section 8.1. A direct link between the volume fraction of reverted austenite and the total elongation in several grades is established in Section 8.2. This allows exploring optimal compositions and processing scenarios for improving the ductility whilst preserving high strength. Concluding remarks are outlined in Section 9.

2. Materials and methods

A number of Fe–Ni–, Fe–Mn–, and Fe–Ni–Mn–based maraging steels were studied following various ageing conditions. Table 1 shows the chemical composition and denomination of the materials tested in this work; experimental results on the microstructure and hardness have been obtained from the literature. The compositional range of these materials will allow to study several microstructural features induced by different alloying elements. The effects of other substitutional elements with less than 1 wt% are ignored due to their low contribution to microstructure evolution. It is worth noting that although the carbon content in most of the steels tested is low, a significant amount of carbides could still be present; this would promote a competition between carbide and intermetallic strengthening. Nevertheless, Schintzer et al. [14,19] and Leitner et al. [3] did not report carbide formation in PH13–8Mo for the ageing conditions employed in this work. Similarly, Zhu et al. [20] did not measure any carbon content in

C300. Additionally, no carbide formation was reported in M350 [21], 5Mn [22], Fe12Ni6Mn [15], LeanLAl and LeanLAl [23], and the Mar6–13 grades [7]. No carbon content in Fe8Ni8Mn was reported [24]. Coarse TiC particles were observed in Lean7Mn, Lean10Mn and Lean12Mn in as-quenched conditions, having volume fraction of 0.22% and a mean size of 500 nm; nevertheless, Qian [25] concluded that they have no influence on hardening due to their size. Similarly, carbide formation in 17–4 SS has been reported [26]; Viswanathan et al. [27] have explored their effects in strengthening, concluding that it is low. Carbide formation in AISI 301 has been reported, however only reverted austenite kinetics is explored in this work. These results show that, for the conditions tested in this work, carbide contribution to strengthening can be ignored. Additionally, except for C300, only Co-free steels are considered in this study, as this work is focused on cost-efficient alloy development. Similarly, it will be assumed that the martensite laths are fully formed in as-quenched conditions and no retained austenite is present, unless otherwise stated; this is to consider a homogenous structure during ageing.

3. Martensite structure

The microstructure of lath martensite in Fe–C steels has been described in previous work [17,18]. The martensite matrix consists of fine lath units (~100–300 nm thick) hierarchically arranged in substructures within the prior-austenite grains (PAG), namely packets and blocks of individual laths. These arrangements accommodate the crystallographic distortions during the transformation from austenite into martensite and ensuring that the net strain in the prior austenite grain is pure dilatation [28]. The packet (d_{packet}) and block (d_{block}) sizes are proportional to the prior-austenite grain size (D_g), where the proportionality constants are determined by the variant number of the austenite/martensite transformation habit planes within an austenite grain and the crystallographic orientation of the laths within a packet, respectively [17]:

$$d_{packet} = \sqrt{\frac{3\sqrt{3}}{8N_p}} D_g = \sqrt{\frac{3\sqrt{3}}{32}} D_g = 0.40D_g, \quad (1)$$

$$d_{block} = \frac{1}{N_b} d_{packet} = \frac{1}{6} d_{packet} = 0.067D_g,$$

where $N_p = 4$ and $N_b = 6$ are the number of packets in a PAG and

Table 1
Chemical composition (in wt%) of the steels tested in this work.

Steel	Ni	Mn	Co	Cr	Al	Ti	Mo	Cu	C	Author
PH13–8Mo	8.2	–	–	12.7	1.1	–	2.2	–	0.03	[3,14,19]
C300	18.8	–	8.5	–	0.12	0.75	4.75	–	–	[20]
M350	18.9	–	0.22	–	0.05	1.9	4.1	–	0.0037	[21]
5Mn	0.3	5	–	–	0.01	–	0.2	–	0.04	[22]
Fe8Ni8Mn	8	8	–	–	–	–	–	–	–	[24]
Fe12Ni6Mn	12	6	–	–	–	–	–	–	0.006	[15]
LeanLAl	1.97	9.1	–	–	0.155	1	1	–	0.0056	[23]
LeanHAl	2.98	8.76	–	–	1.33	–	–	–	0.01	[23]
Lean7Mn	2	7	–	–	1	1	1	–	0.03	[25]
Lean10Mn	2	10	–	–	1	1	1	–	0.015	[25]
Lean12Mn	2	12	–	–	1	1	1	–	0.02	[25]
AISI 301	6.5	1.29	–	17.3	–	–	–	–	0.11	[83]
17–4 SS	3.94	0.52	–	16.24	–	–	–	3.3	0.049	[26]
Mar6	2.5	0.5	–	–	0.6	–	–	2.5	0.06	[7]
Mar7	2.5	1.5	–	–	0.5	–	–	2.5	0.06	[7]
Mar9	4	1.5	–	–	1	–	–	2.5	0.05	[7]
Mar11	4	3	–	–	1.5	–	–	3	0.05	[7]
Mar13	4	4	–	–	1	–	–	4	0.05	[7]

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