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Computer simulation of the yield strength evolution in Cu-precipitation strengthened ferritic steel

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ABSTRACT

During ageing of steel containing a few percent Cu, a maximum increase of hardness and strength can be observed after several hours of annealing at around 500–550 °C. This strength increase is caused by small coherent bcc-Cu-precipitates of 2–3 nm diameter. For consistent computer simulations of the early stages of precipitation, it is shown that variations in the equilibrium Fe-content of the bcc-Cu nuclei must be taken into account. The simulated precipitation parameters are compared to experimental data reported in literature. Good agreement between experiment and simulation can be achieved in terms of the evolution of phase fraction, number density and mean radius of the Cu-precipitates. Based on these results, different models for precipitation strengthening are assessed and their predictions compared to the experimentally observed strength evolution. We find that mainly the coherency strain and modulus strengthening effects contribute to the precipitation strengthening potential. Together with the intrinsic strength of the alloy and Cu solid-solution strengthening, a consistent description of the lower yield strength evolution during precipitation hardening of an Fe–1.4% Cu alloy is achieved.

1. Introduction

The kinetics of Cu-precipitation in steel was subject to several experimental as well as numerical analyses, e.g. [1–6]. Therefore, morphology, crystallography and kinetics of Cu-precipitation in α-iron are well documented. It is generally accepted that, in the early stages of ageing, Cu-precipitates undergo a multi-stage transformation from coherent body centred cubic (bcc) to incoherent face centred cubic (fcc) structure. During this evolution, a change in the chemical composition of the Cu-precipitates with respect to the Fe-content can be observed. The exact amount of Fe in the early bcc-Cu-precipitates is still a topic under discussion, as concluded by Fine et al. [6]. These authors point out that, considering experimental results obtained by atom probe analysis, a significant amount of Fe can be detected in the Cu-precipitates. In contrast, positron annihilation and neutron scattering studies suggest compositions close to pure Cu. Also, numerical analyses are inconclusive with conflicting results [7,8]. In a recent theoretical study [9], evidence is provided towards the assumption that finely dispersed Cu-precipitates in the very early stages of ageing contain a significant amount of Fe.

The dense distribution of coherent bcc-Cu-precipitates leads to a distinct increase in strength and hardness, where the peak strength condition coincides with the maximum precipitate number density. At this point, the mean diameter of the precipitates is approximately 2–3 nm. Depending on ageing conditions, this maximum is often observed after several hours [10,11], followed by a pronounced decrease in number density during overageing with a simultaneous decrease in strength. Interestingly, this drop in number density cannot be described by classical Ostwald ripening theory alone due to the fact that the reduction in number density predicted by this theory would be several orders of magnitude too slow.

This discrepancy has stimulated detailed numerical investigations and the development of a simulation methodology, which differs from conventional approaches reported in literature [11–13] by taking into account compositional variations of the critical nucleus. In the present approach, the actual composition of the nuclei is evaluated based on the concept of a minimum nucleation barrier [2,9]. It is demonstrated that these initial variations have huge impact also on the further precipitate evolution.

From the example of an Fe–1.4 at.% Cu alloy, which was investigated experimentally by Goodman et al. [1] during ageing at 500 °C using field ion microscopy (FIM) and transmission electron microscopy (TEM), the theoretical precipitation strengthening potential is evaluated based on different strengthening models. Together with the intrinsic strength of the alloy and the solid-solution strengthening effect by Cu, the lower yield strength evolution during a precipitation hardening treatment is evaluated.

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The results are found to be in good qualitative and quantitative agreement with the experimental values.

2. Numerical simulation of Cu-precipitation

2.1. Simulation of Cu-precipitation in α-iron

All simulations carried out in this work are performed with the software MatCalc [14–17] version 5.30.1096. The thermodynamic and diffusion data are compiled from the assessments of Turchanin et al. [18] and Fridberg et al. [19], respectively. The energy of the precipitate/matrix interface γ_0 is calculated from the generalized broken-bond (GBB) approach [20] for planar, sharp interfaces, which delivers reasonable estimates for the chemical component of the interfacial energy. The precipitate size effect on the interfacial energy is taken into account by a radius-dependent correction factor [21]. In addition, the impact of atomic mixing at the precipitate/matrix interface (entropic effects, see e.g. Ref. [22]) is taken into account with a constant correction factor of 0.9. Due to the small volumetric misfit of the coherent Cu-precipitates [1], the elastic strain energy per unit volume of a particle was neglected when calculating the critical nucleation energy. Further kinetic effects of, e.g. quenched-in vacancies, are taken into account in the diffusion coefficient by a constant factor of 150. No other fitting parameters are used in the simulations.

Previous applications of the present approach to precipitation in a complex tool steel [23] and a Ni-base superalloy [24] have been reported earlier. These papers contain supplementary details on the simulation procedure [16].

2.2. Simulations with constant nucleus composition

The time-dependent nucleation rate J is given by classical nucleation theory [25] with

$$J = N_0 Z \beta^* \cdot \exp\left(\frac{-G^*}{k \cdot T}\right) \cdot \exp\left(\frac{-\tau}{t}\right). \quad (1)$$

J describes the rate at which new nuclei are created per unit volume and unit time. N_0 represents the total number of potential nucleation sites, Z is the Zeldovich factor, β^* is the atomic attachment rate, k is the Boltzmann constant, T is temperature, G^* is the critical nucleation energy, τ is the incubation time and t is time.

In multi-component alloys, it is generally assumed that supercritical precipitate nuclei adopt the particular chemical composition, which yields the maximum driving force (ortho-equilibrium composition) for precipitation. With this criterion, the otherwise undetermined Fe- and Cu-content of the nucleus can be fixed and the individual terms in Eq. (1) can be evaluated. In the present case, the ortho-equilibrium criterion implies that the nuclei consist of practically pure Cu. With Eq. (1) and application of a suitable growth law, see e.g. Refs. [15,26], the further evolution of the supercritical nuclei is fully determined. Here, the time integration of the evolution equations is performed in the framework of the numerical Kampmann–Wagner approach [27] as described in detail in Ref. [16]. Similar approaches have been reported by e.g. Hutchinson et al. [11] and Perez et al. [13] for Cu-precipitation in α-iron, or by Myhr et al. [28,29] and Nicolas and Deschamps [30] in Al-alloys.

In order to reproduce the experimental results of Goodman et al. [1], numerous simulations have been carried out in the MatCalc software with parameter variations in the interfacial energy and diffusional mobility. Exemplary results of such variations are shown in Fig. 1(a)–(c), where the calculated sharp interface energy γ_0 is varied with multiplicative pre-factors. Interestingly, no combination of simulation input parameters could be found, which lead to a consistent representation of the experimentally measured precipitation kinetics. With any variation of parameters (interfacial energy and diffusional mobility) and assuming that the critical bcc-Cu nucleus has ortho-equilibrium chemical composition, it has only

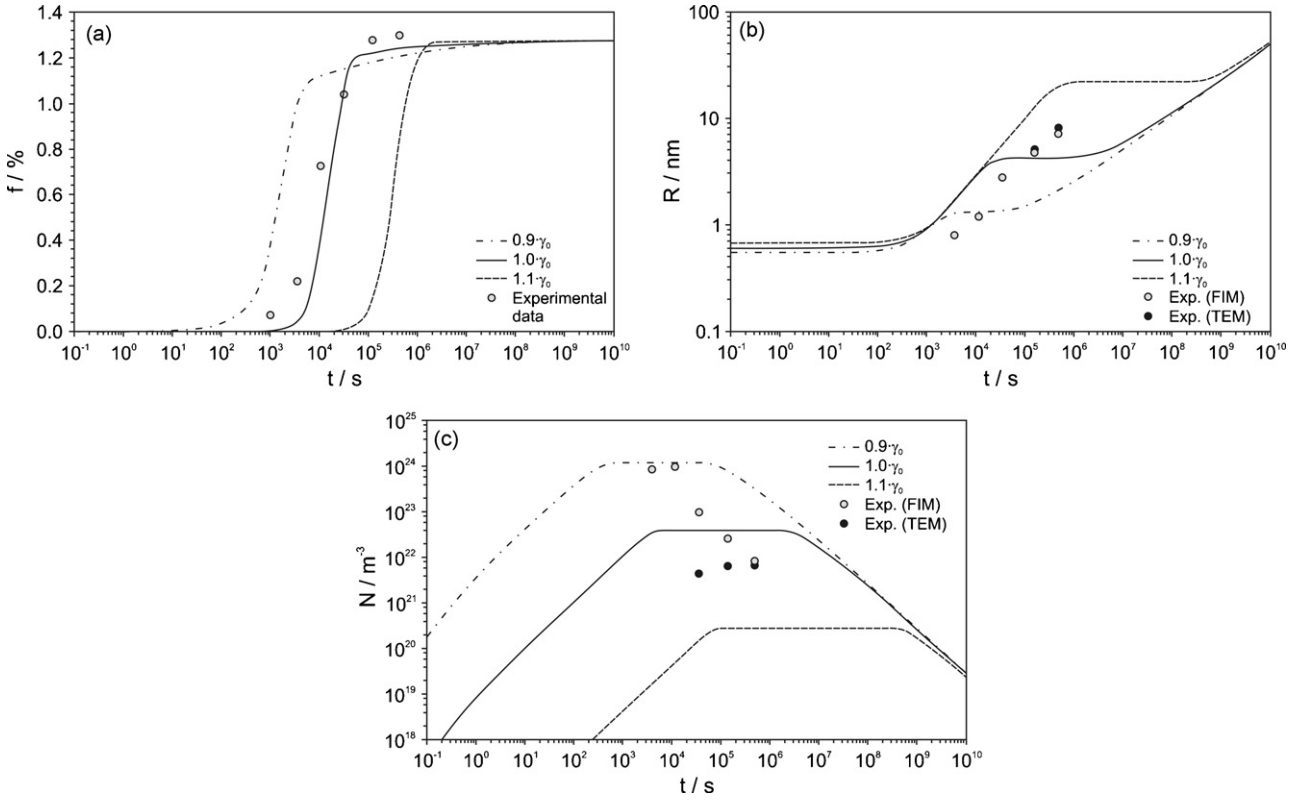

Fig. 1. (a)–(c) Calculated evolution of phase fraction (f), mean particle radius (R) and number density (N) for bcc-Cu-precipitates with ortho-equilibrium nucleus composition. The different lines in each plot show the result of a parameter variation of the interfacial energy (γ_0).