A study of composition and annealing temperature influence on the mechanical properties of Fe-Cr-Al alloys

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Abstract

In this work, phase-field modeling of externally applied mechanical loading to ternary Fe-Cr-Al alloys was performed in order to study the influence of alloy composition and annealing temperature on the changes in their mechanical properties. For sample preparation we exploited a generalized model of the phase field with CALPHAD approach. Using the combination of the phase field method with the nonlinear elasticity theory, which was proposed in references [1-3], the simulation of plastic deformation of Fe-Cr-Al alloy samples was performed. Such approach makes it possible to describe the elastic fields redistribution, particularly elastic strain and stress, under mechanical loading. In this work we investigated processes of plastic deformation in the form of simple shear with constant strain rate $10^9 s^{-1}$.

Introduction

Despite significant progress in experimental and theoretical researching of material properties of iron-based Fe-Cr-Al alloys for use in nuclear applications for a wide range of compositions, one of the open questions related to prediction the mechanical properties of these alloys remains actual. Moreover, a study of elastic fields evolution and defects dynamics under mechanical loads conditions is necessary to establish complete information about the physical mechanisms of hardening, that is important for further composition design and predicting of alloy durability and reliability.

Main tasks are:

1. To perform numerical simulations of mechanical loading, applied to iron-based Fe-Cr-Al alloys with different content of alloying elements (Cr and Al), which were annealed at different temperatures.
2. To calculate the stress-strain diagrams for previously obtained alloy samples at shear deformation.
3. To determine the mechanical characteristics and analyze the alloying elements and annealing temperature effect onto the strength.
4. To obtain the distributions of elastic strains and stresses.
5. To study the formation and evolution of the slips.

The Model

General form of the Gibbs free energy

$$\mathcal{G} = V_m^{-1}\int_V \left[G_{ch}(\{x_\mu\},\{c_d\}) + G_\nabla(\{\nabla x_\mu\},\{\nabla c_d\}) + G_{el}(\mathbf{u},x_\mu)\right] \mathrm{d}\mathbf{r} \quad (1)$$

G_{ch} – relates to molar Gibbs free energy and point defects
G_∇ – gradient energy term
x_μ – concentration fields ($\mu = \{Fe, Cr, Al\}$)
c_d – concentration of point defects ($d = \{i, v\}$, i – interstitials, v – vacancies); $\mathbf{u} = (u_x, u_y)$ – elastic displacement vector

Elastic energy

$$G_{el}(\mathbf{u},x_\mu) = \frac{1}{2}Ke_1^2 + \Phi(e_2,e_3) + \alpha e_1 x_\mu \quad (2)$$

$$\Phi(e_2,e_3) = \frac{\nu}{8\pi^2}\left[1 - \cos\pi(e_2+e_3)\cos\pi(e_2-e_3)\right] \quad (3)$$

Elastic strain components:

$$\begin{aligned} e_1 &= \nabla\cdot\mathbf{u} && \text{– dilation strain}\\ e_2 &= \nabla_x u_x - \nabla_y u_y && \text{– tetragonal strain}\\ e_3 &= \nabla_y u_x + \nabla_x u_y && \text{– shear strain}\end{aligned} \quad (4)$$

Elastic moduli:

$$\begin{aligned} K &= \textstyle\sum K_\mu x_\mu && \text{– bulk elastic modulus}\\ \nu &= \textstyle\sum \nu_\mu x_\mu && \text{– shear modulus}\end{aligned} \quad (5)$$

The Model

Dynamics of the composition and defect concentrations fields:

$$\partial_t x_{Cr} = \nabla\cdot\left[M_{CrCr}\nabla\frac{\delta\mathcal{G}}{\delta x_{Cr}} + M_{CrAl}\nabla\frac{\delta\mathcal{G}}{\delta x_{Al}}\right] \quad (6)$$

$$\partial_t x_{Al} = \nabla\cdot\left[M_{AlAl}\nabla\frac{\delta\mathcal{G}}{\delta x_{Al}} + M_{CrAl}\nabla\frac{\delta\mathcal{G}}{\delta x_{Cr}}\right] \quad (7)$$

$$\partial_t c_v = \nabla\cdot L_v\nabla\frac{\delta\mathcal{G}}{\delta c_v},\quad \partial_t c_i = \nabla\cdot L_i\nabla\frac{\delta\mathcal{G}}{\delta c_i} \quad (8)$$

M_{CrCr}, M_{AlAl}, M_{CrAl} – mobility coefficients
L_v, L_i – mobility for the vacancies and interstitials

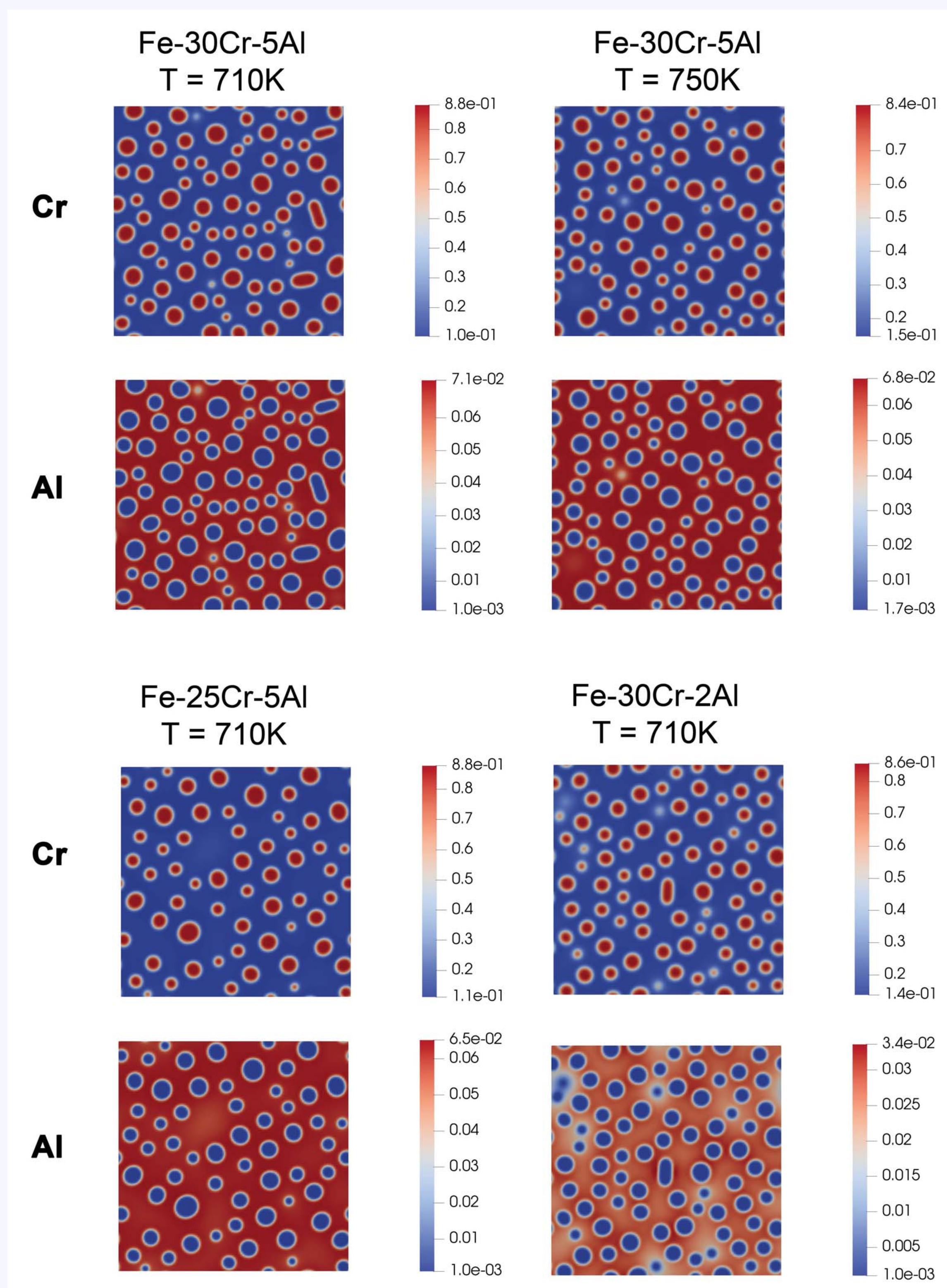
Dynamics of the elastic fields

$$\rho\frac{\partial\mathbf{v}}{\partial t} = \eta_0\nabla^2\mathbf{v} + \nabla\cdot\overleftrightarrow{\sigma} \quad (9)$$

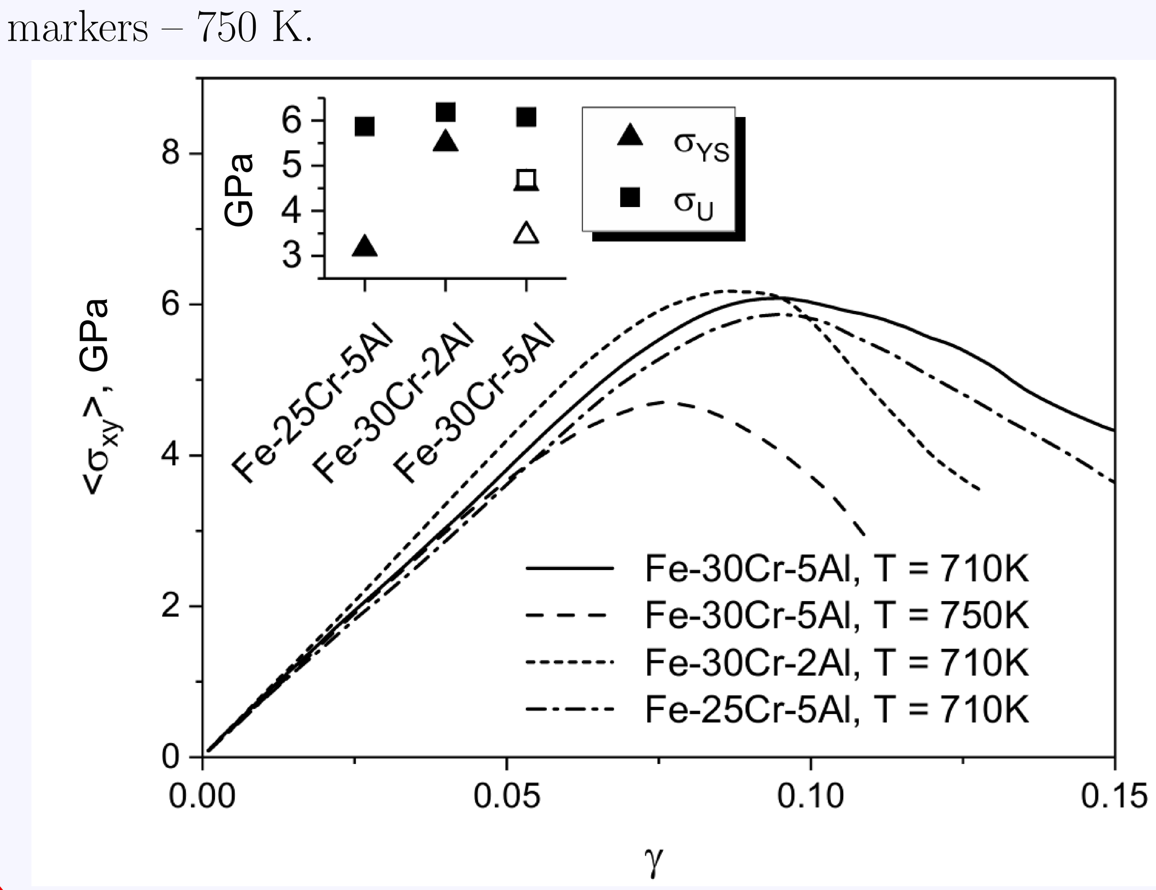
$\mathbf{v} = \partial\mathbf{u}/\partial t$ – lattice velocity, ρ – mass density, η_0 – shear viscosity, $\overleftrightarrow{\sigma} = \{\sigma_{ij}\}$ – elastic stress tensor ($\nabla\cdot\overleftrightarrow{\sigma} = -\delta\mathcal{G}/\delta\mathbf{u}$)

Simulations

Composition of ternary Fe-Cr-Al alloys



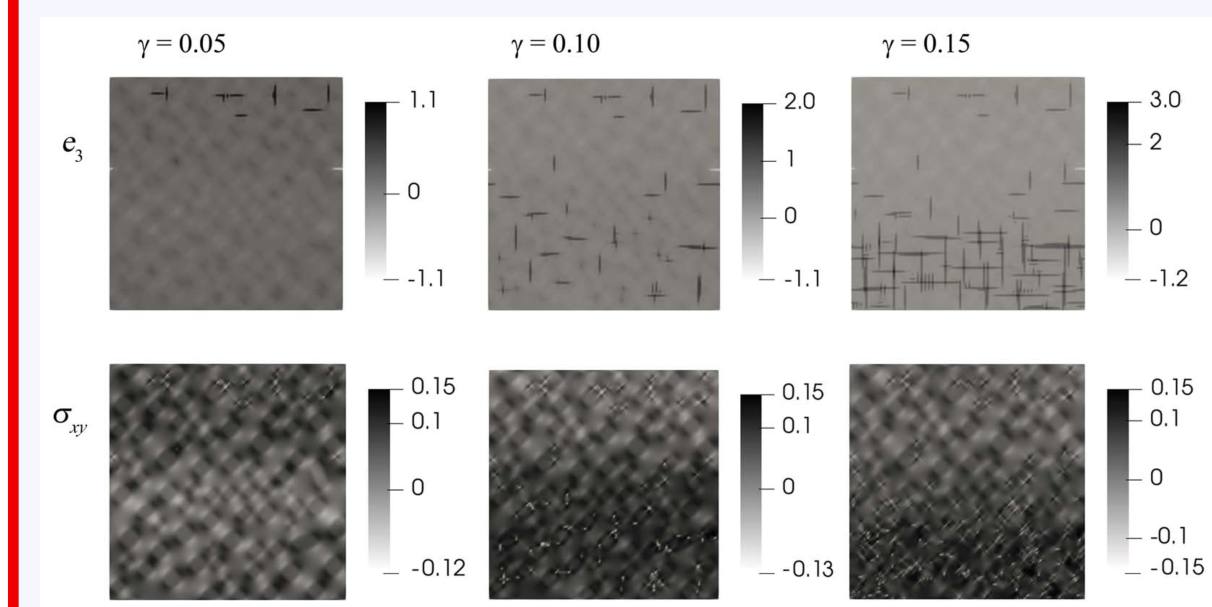
Stress-strain curves for shear deformation γ with constant strain rate $\dot{\gamma} = 10^9 s^{-1}$ The corresponding values of yield strength σ_{YS} and ultimate strength σ_U are shown in the inset. Closed markers correspond to temperature 710 K, open markers – 750 K.



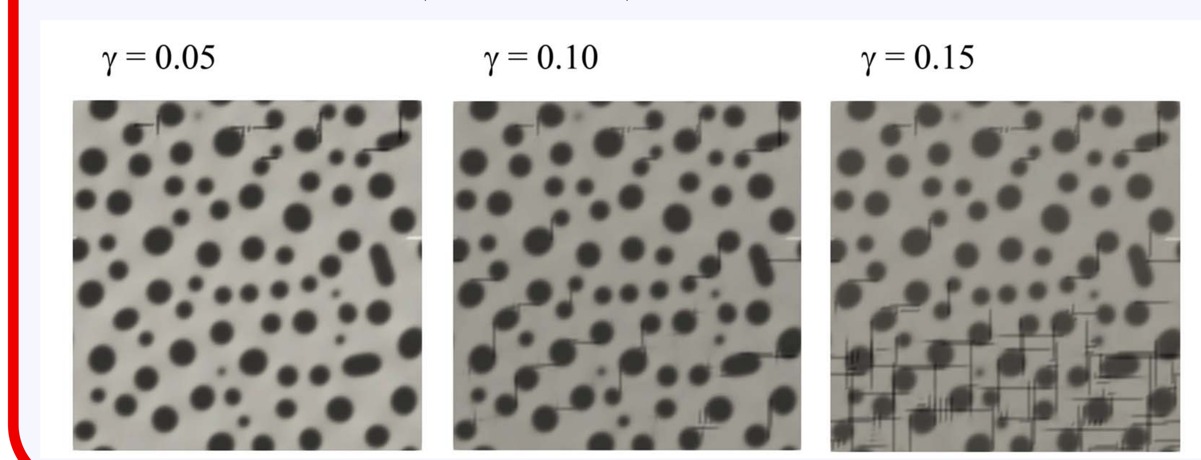
Simulations

Elastic fields evolution for Fe-30Cr-5Al alloy sample annealed at $T = 710$ K.

Distributions of elastic deformations e_3 and shear stress σ_{xy} fields during shear loading in time points at $\gamma = 0.05; 0.10; 0.15$, which correspond to solid deformation curve. Snapshots of e_3 demonstrate the formation of slip lines. Average values of σ_{xy} field relate to corresponding deformation curve.



Distribution of slips together with Cr composition in the sample of Fe-30Cr-5Al alloy ($T = 710$ K) under shear.



Conclusions

The analysis of the obtained data showed that mechanical properties take higher values at lower annealing temperature, higher Cr content and lower Al content. We have found that:

- a decrease in temperature from 750 K to 710 K leads to an increase in yield strength and ultimate strength by 33.5% and 42.4%, respectively.
- an increase in Cr content from 25% to 30% (at 5% Al content) leads to the increase in yield strength and ultimate strength by 45.8% and 3.5%, respectively. At the same time the increase in Al content from 2% to 5% (at 30% Cr content), in contrast, results in the decrease in yield strength and ultimate strength by 19.1% and 1.8%, respectively.

Thus, the decrease of the annealing temperature, decrease of the Al content and increase of Cr content result in growth of the material resistance to plastic deformation and strengthening of Fe-Cr-Al alloy.

It was shown, that slips, which are the fundamental flow units in plastic deformation in considered model, are mainly located around chromium-enriched precipitates in the softer (matrix) phase, whereas their edges are mostly trapped at interfaces.

Obtained results are consistent with the general trends from both experimental investigations and simulations [4–8].

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