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The effect of size of Cu precipitation on the mechanical properties of microalloyed steel

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ABSTRACT

The effect of size of nanoscale Cu precipitate on the mechanical response of microalloyed steel was investigated computationally and experimentally. A phenomenological constitutive description is adopted to build the computational crystal model. The material is envisaged as a composite; the Cu precipitate is modeled as a monocrystalline core surrounded with a lower yield stress and higher work hardening rate response. Both a quasi-isotropic and crystal plasticity approaches are used to simulate the matrix. The nanoscale precipitate is modeled as ellipsoidal inclusion with different Yound's modulus to matrix. Elastic and plastic anisotropy are incorporated into this simulation. An implicit Lagrangian finite element formulation with von Mises plasticity or rate dependent crystal plasticity is used to study the nonuniform deformation and localized plastic flow. The computational predictions are compared with the experimentally determined mechanical response of HSLA-100 steel with average size of nanoscale precipitates of 2.02 ± 1.89 nm. The tendency of the calculated yield strength attributed to Cu precipitates is in good agreement with experimental result.

1. Introduction

Macroscopic properties, such as yield stress, ductility and toughness, are the key criteria in choosing a material for engineering applications. In principle, the macroscopic properties of a material are determined by its microstructure. For the microalloyed steel, the overall behavior is strongly depends on the type, size and distribution of various phases in the material [1–4], as well as the grain size [5,6]. Thus, building a link between the microstructure and the macroscopic properties of the microalloyed steel is essential to design a preferred microstructure, which contains the desired properties for specific engineering applications. In recent papers, a multi-scale micromorphic model for hierarchical materials, which has been used successfully on the multi-scale character of damage and failure in steel possessing particle distributions at two distinct scales [7,8]. The model can be used to describe a material containing an arbitrary number of scales of microstructure and opens the door for the modeling of a range of materials possessing a hierarchical microstructure. However, when implementing the model in the finite element method, the element size is required to be on the order of the smallest microstructural length scale, which can result in very expensive (time and cost) simulation on large domains [8].

Low-carbon copper-bearing age-hardenable high strength low alloy (HSLA) steels are a class of HSLA steels which provide good combinations of strength, low temperature toughness and weldability. The strength level of the copper-containing steels can be improved by age hardening, and such steels have been developed for naval and defense application [9]. The morphology of copper precipitates in proeutectoid ferrite has been examined in previous work [10]. Most of the elements provide hardenability for the transformation of austenite to a fine bainitic ferritic microstructure in heavy sections. In addition, the presence of Cu contributes to precipitate hardening by copper rich particles during aging[11] as well as promoting good deformability without losing ductility[12], excellent corrosion resistance[13], and high resistance to fatigue crack growth because of crack path obstacles in the form of fine copper-rich particles[14]. The most significant effect of Cu precipitates in steel is size control [15], which directly influences mechanical properties. The size of Cu precipitates fluctuates over a large range, from several nanometers to several tens of nanometers, according to chemical composition, heat treatment, and steel processing conditions [16]. In the context, Cu precipitate has been studied by numerical and experimental methods. However, some numerical methods can result in expensive simulation in large domain. In addition, it is different to trace the performance of Cu precipitate in microalloyed steels by the experimental method.

The purpose of this paper is to study the effect about size of Cu precipitates on the mechanical properties of low carbon HSLA steels by finite element method (FEM). In this FE model, the simulation

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domain is simplified, which includes Cu precipitates dispersing and the matrix. The FEM results of the effect of size of Cu precipitation are compared with the experimental results.

2. Finite element model

The deformation behavior of microalloyed steel including Cu precipitates strongly depends on the size of Cu precipitation. The evolution of the size of the anisotropic yield surface is described with the isotropic hardening while its macroscopic translation via kinematic hardening is formulated according to the initial structure of the precipitates of the alloy [17]. While the influence of size of second phase particles on the flow stress is well known, the effect of the precipitates on the strength at the initial and deformed state has not been thoroughly investigated.

2.1. Constitutive model

The simulation of material behavior considers 2 effects; each has to be characterized by a macroscopically measurable variable

1. kinematic hardening, dislocation evolution, internal stress σ_i;
2. precipitation strengthening, particle stress σ_p.

The flow response depends highly on the development of the internal changes in the material's microstructure. The total strain rate is assumed to be separable into internal and precipitate strains. It should be noted that the dislocations are the most important internal variable measure. In addition, more parameters are required for a full characterization of the microstructure, e.g. grain size and shape, second phase fractions, precipitate morphology, etc. In order to simplify the constitutive model, the flow rate is described as a function of not only external influences such as applied stress level, but also of internal factors, as characterized by I in Eq.(1)

$$\dot{\varepsilon} = \dot{\varepsilon}(\sigma, I) \tag{1}$$

The material law applied is based on the over-stress conception considering internal changes of the microstructure (Eq. (2))

$$\dot{\varepsilon}_{ij} = \dot{\varepsilon}\left[\sigma_{ij} - (\alpha_{ij}^{\text{int ern}} + \beta_{ij}^{\text{intern}})\right]^N = \dot{\varepsilon}\sigma_{ij}^{\text{over}} \tag{2}$$

where α_{ij} and β_{ij} represent the kinematic work hardening and influence of precipitation, respectively.

The hardening behavior of flow mechanisms is assumed to be kinematic. Based on a proposal by Kocks and Mecking [18], the evolution equation of the dislocation density ρ can be written as

$$\frac{d\rho}{d\varepsilon} = M\left[k_1\sqrt{\rho} - k_2\rho\right] \tag{3}$$

The kinematic work hardening term, with regard to the overstress concept, is assumed to be proportional to the square root of the dislocation density [19].

$$\hat{\sigma} = CGb\sqrt{\rho} \tag{4}$$

where G and b are shear moduls and Burger's vector, respectively. C is a constant from 0.2 to 0.4.

The simulation of the influence of Cu precipitates on the mechanical behavior requires a theory which considers the precipitate-dislocation interaction. The relationship between the properties and the microstructure involves the relationship between the precipitate size and the interparticle spacing of the dispersed phase. For the present simulation it is assumed that yield stress of precipitate-hardened material, is controlled by the local crossing of dislocations over the precipitates [20]. For small to moderate strains, the precipitate is usually assumed not to be subjected to plastic strain. The averaged stress of the precipitate σ_p is, therefore, assumed to be reversible and reflects here the back stress term. With significant higher yield stresses in the precipitates than in the lattice, high dislocation densities can be expected in the close neighborhood of the precipitates. Precipitates are known to induce also higher initial values in the critical resolved shear stresses which can be explained by bowing of dislocations.

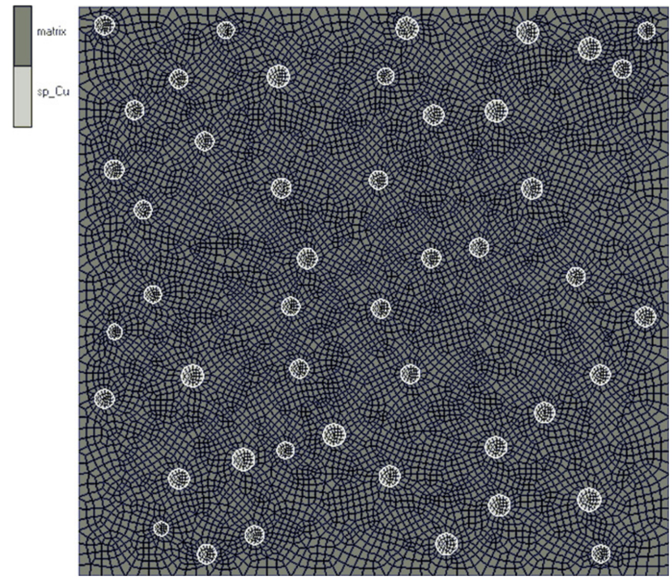

Fig. 1. FE model of two phases in MSC.Marc.

Table 1
Simulation parameters of two phases.

	E (GPa)	ν	φ (%)	G (GPa)	C	b (10^{-9} m)	Flow stress curve
Cu precipitate	160[21]	0.326	5	60.3	0.3	0.35	Eq. (4)
Matrix	210	0.3	95	80.8	0.3	0.29	Eq. (4)

2.2. Simulation procedure

To investigate the performance of Cu precipitate in microalloyed ferrite steel under plastic deformation, two phase model was constructed by finite element method as shown in Fig. 1. In this simulation, the part of grain was studied due to the nanoscale precipitates. The stress in each of the two components of the composite is calculated using the assumption that the strains in both phases are the same and are equal to the macroscopic applied strain and the precipitation directly combines with the matrix. In the simulation model, the average size of Cu precipitates is 2.5, 5 and 10 nm. In addition, the standard deviation of precipitation size is 0.394, 0.788 and 1.576 nm. In the present work, material properties and fraction of precipitates are given in Table 1. The quantity E denotes the Young's modulus, ν denotes the Poisson ratio, and φ is volume fraction of precipitate and matrix. The flow stress curves of the two phases are expressed by Eq. (4), in which C, G and b are used.

3. Results and discussion

With the aid of the above computational model, a large-scale 2D multi continuum simulation of the tensile process with