

CuO/Cu<sub>2</sub>O/Cu/Cu<sub>3</sub>Ti<sub>3</sub>O/Cu<sub>3</sub>TiO<sub>4</sub>, Fe<sub>2</sub>O<sub>3</sub>/FeO/Fe/ZrO<sub>2</sub> и CuO/Cu<sub>2</sub>O/Cu/ZrO<sub>2</sub>. Образующиеся частицы имеют ламинарно-глобулярную структуру состава механокомпозит/оксид. Композиционные гранулы Cu/Zr-CuO и Fe/Zr – Fe<sub>2</sub>O<sub>3</sub> имеют больший размер гранул (до 60 и 40 мкм соответственно), чем при легировании титаном (до 40 и 25 мкм соответственно).

Применение механокомпозиционных порошков Fe/Me и Cu/Me в качестве восстановителя в реакциях с оксидами позволяет снизить активность металлов циркония и титана, что обеспечивает возможность управления кинетикой фазообразования в системах Cu/Me–CuO и Fe/Me–Fe<sub>2</sub>O<sub>3</sub>.

Наблюдаемые различия в кинетике фазо- и структурообразования в условиях интенсивной механической активации могут быть связаны с различием типа кристаллических решеток меди (ГЦК) и железа (ОЦК) и, следовательно, различием типов генерируемых дефектов в процессе нагружения и сдвиговых деформаций.

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## MODELING OF PRECIPITATION KINETICS OF MANGANESE AND COPPER SULFIDES IN INTERSTITIAL FREE STEELS

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Low carbon steel production with copper sulfide precipitation strengthening is being now extensively investigated owing to its lower cost as compared to that with steelmaking using Nb and Ti precipitates. Copper is always available in steel scrap. In some cases steels with copper sulfide precipitates have even better mechanical properties than those with Nb/Ti precipitates. Currently such low-carbon steels with high mechanical properties are under active investigation. Precipitation hardening and strengthening have a great effect on mechanical properties of these steels.

Precipitation kinetic is modeled on the basis of classical nucleation and growth theory (CNGT).

The different numerical schemes and details are presented in [1]. For many cases the modeling of homogeneous nucleation and growth by CNGT gives satisfactory agreement with experimental data. In some cases fitting of parameters is not used at all, in others one or two parameters are fitted. But as a rule even in the latter cases good agreement is observed for a great num-

ber of temperature regimes and initial concentrations of solutes as well as for multi-component and multi-phase precipitation.

By now the physical nature of heterogeneous nucleation of copper sulfides is practically unknown. There are many hypotheses about heterogeneous nucleation sites for CuS including grain borders, matrix-MnS inclusion interfaces, dislocations, Cu or S microsegregation and so on. In general, the method considered can be used for describing various models of nucleation, by means of simultaneous following both MnS and Cu<sub>2</sub>S nucleation. In this work the assumption is made that precipitations of copper and manganese sulfides are independent. Next we assumed that the diffusions of copper, manganese and sulfur atoms are independent as well.

The only one available work devoted to approximate modeling of copper sulfides precipitation kinetic is presented in [2]. We shall model precipitation using approximately the following composition: copper is 0.07 wt%, sulfur 0.04 wt% and manganese concentration 0.54 wt% for steels with hot and cold rolling.

The considerations accepted here to be used for simulation of precipitation kinetics on the basis of CNGT are as follows:

1. Wholly diffusion-controlled precipitation is assumed for our case on the basis of spherical shapes of inclusions and reported cube-cube orientation between copper sulfide inclusions and matrix [2].

2. All heterogeneous nucleation sites have deformed lattice around nucleation sites and hence have higher mobility of Cu atoms as compared with that in ideal matrix. In this work the model of Cu diffusion near dislocations has been selected for nucleation and initial growth modeling. The characteristic feature of this model is that in the temperature range 200 to 500°C the Cu diffusion coefficient may be a few orders of magnitude higher than this coefficient in ideal matrix.

In [3] the thermodynamic calculation resulted in obtaining the dependence of driving force for Cu<sub>2</sub>S on temperature. The equilibrium temperature is about 740 °C for 0.0015C–0.2Mn–0.06Si–0.01S–0.06P–0.02Nb–0.05Cu–0.035Al (wt %) steels assuming the absence of sulfur reactions with manganese and iron.

The equilibrium temperature may depend on initial solute concentration, phase transition parameters and others. An insignificant error made in experimental measurement of copper solubility in matrix may actually lead to substantial deviation from correct equilibrium temperature. This inaccuracy is less important for estimation of phase transition enthalpy. On assumption that solubility product depends only on temperature end the enthalpy estimated as in [2]. The equilibrium temperature for 0.05%Cu and 0.01%S is estimated as 740 °C according to [3].

The equilibrium concentrations  $c^i$  of solutes in matrix at the matrix-precipitate boundary are increased owing to the curvature of surface between matrix and precipitate. It is assumed that the inclusion has spherical shape with current radius  $R$ . As to binary alloys new solute equilibrium concentration is defined by precipitate radius.

The average precipitate radius is little dependent on critical radius for sufficiently long time of precipitation, but activation barrier, precipitation rate and inclusions density may considerably depend on critical radius.

This model describes homogeneous nucleation. As to heterogeneous nucleation some parameters in equations must be modified. The heterogeneous nucleation of Cu<sub>2</sub>S is expected to be mainly located on dislocations as soon as the density of dislocations rises to high values following hot and cold rolling.

The significant feature of growth on dislocations is rapid diffusion of copper atoms in a small zone around dislocation. In order to exactly consider this phenomenon the conception of depleted zone is introduced [4, 5].

The solute balance equations are used for estimation of current concentrations of Cu and S. In this approximation it is assumed, that the solute fraction distribution is uniform in matrix.

N– model [6] will be used for describing the evolution of precipitate size distribution. In this model the particle size distribution function (PSD) is discretized into  $N_c$  number of size classes. The class is defined by radius  $R_i$  and the number of inclusions with radius size between  $R_i - \Delta R/2$  and  $R_i + \Delta R/2$ .

In case of using “Euler like” method for calculation the boundaries of classes are fixed and fluxes of particles between classes are estimated. The details are presented in [1].

The initial distribution for  $N_i$  is null or known (for example experimental data) distribution.

The adaptive step time  $\Delta t$  is used because the radius change during  $\Delta t$  time has not been above  $\Delta R/2$ . This limitation eliminates the possibility to “jump” across one or more classes. The maximum speed  $v$  has classes with small  $R$ .

New size classes are created for high  $R$  values during inclusion growth. And quite the contrary, if the number of particles in a class with small radius is less than 1 it will be excluded from calculation. This makes it possible to increase step time  $\Delta t$  and to calculate particle growth during long annealing periods.

### Conclusions

Model for nucleation and growth the precipitation of manganese and copper sulfides inclusions are developed. New estimation of Gibbs free energy change for precipitation of copper sulfides is used. Model of nucleation and growth of copper sulfides precipitates on dislocations are used for heterogeneous nucleation. Numeric model, based on “Euler like” method, are developed for calculations.

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## ТЕРМОКИНЕТИЧЕСКАЯ ЭДС В СПЛАВЕ TiNi ПРИ ПРЯМОМ ФАЗОВОМ ПЕРЕХОДЕ: ЭКСПЕРИМЕНТ И РАСЧЕТ

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Примером возникновения термокинетической ЭДС в однородных материалах служит наведение ЭДС в результате перемещения зоны нагрева вдоль проволочного железного образца. Причиной возникновения такого рода термокинетической ЭДС является реализация фазового превращения в локальной зоне нагрева при температурах 700–800 °С [1]. В ряде материалов фазовые превращения могут протекать при значительно более низких температурах, например, в сплавах, обладающих эффектом памяти формы. При реализации термоупругих фазовых превращений инициирование ЭДС в этом случае возможно