COMPUTER MODELING OF INFLUENCE OF PREVIOUS DEFORMATION DEGREE AND STRAIN RATE ON CARBONITRIDES PRECIPITATION KINETICS IN LOW-CARBON MICRO-ALLOYED STEEL

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Abstract: *Using computer modelling with originally developed semi empirical physical grounded models a study was carried out to investigate influence of previous hot deformation on carbonitrides formation from austenite in low-carbon micro-alloyed steel. Studied in the article is an influence of degree and rate of the deformation on processes of nucleation and growth of Nb and Ti carbonitride particles. The model helps to predict not only process of changing in number and average size of the particles but also to estimate their final size distribution. One of additional peculiarities of the developed model is its ability to predict composition of the cabinetries formed in certain conditions. The model takes into account process of recrystallization and returning, which affect carbonitrides precipitation and are influenced by it. Acceleration was shown of both nucleation and growth rates of the particles due to increasing of deformation degree and strain rate. Another result is that previous deformation significantly affects size distribution function of the particles precipitated with rather lesser effect on their average size. Kinetic curves and final size distribution plots are given.*
KEYWORDS: *STEEL, CARBONITRIDES, MODELLING, DEFORMATION*

1. Introduction

The *objective* of the research is to demonstrate the developed model ability in prediction of processes of carbonitrides precipitation and show an influence of deformation on the particles size distribution.

Precipitation from solid solution (austenite) of carbonitride phases occurs in steels micro alloyed with Ti, Nb, V and Zr. Stimulating for the precipitation is previous deformation, which leads to increase in inner stress and dislocation density of the material. But owing to high temperature of the processes there have a place phenomena of returning and recrystallization [1].

A mathematical model and sufficient computational program was developed to describe kinetics of carbonitrides precipitation from austenite after deformation. The model takes into account returning and recrystallization their influence on carbonitrides nucleation and vice versa. Detailed description of the model can be found in our previous work [2], some information is also in our book [3] (in chapter 1). Here we do not consider on the essence of the model and its realization. It is a semienpirical but physical based model. Finite differences method was used for realization of the processes calculation.

Successful enough preempts were made before to describe theoretically kinetics of recrystallization and carbonitrides precipitation in deformed steel [4-6]. Even a program was developed [4], but it is not an open source. So program code realization for the model implementation was made originally by us. A remarkable feature of our model, qualitatively distinguishing it from the above one is including of thermodynamic calculation of the carbonitrides composition. For instance in the work [4] they consider carbonitrides as stoichiometric composition, which is a rather rough approximation and does not correspond to the composition of real inclusions. As a bases of thermodynamic module for carbonitrides composition calculation was taken our previously developed program. It was completely rewritten using Python language (original was in Delphi), program code optimization were made and precision increased (the nonideality of carbonitride as a mutual solid solution of the corresponding carbide and nitride is better taken into account). Another feature of current investigation is consideration on size distribution of the cabinetries precipitated. In particular the influence of deformation degree and strain rate on the particles size distribution was studied using the model developed. In other papers known to us, the average indicators were modeled and investigated, but not the distribution functions. There are many others lesser particularities our model consisting in a more accurate consideration of many quantities and their dependencies but their description will lead to detail that make it difficult to understand.

2.1. Studied material

Chemical composition of the studied steel in this work is given in table 1.

Table 1

Chemical composition of the studied steel

Fe	C	Mn	Si	Mo	Ti	V	Nb	N
base	0.10	2.00	0.25	0.15	0.015	0.02	0.045	0.006

The given composition is quit similar to one from our work [2] but amounts of Mn an Mo are higher and concentration of carbon is lesser. It’s seen that the steel is low-carbon one and has rather high amount of Mn. It is micro alloyed with strong carbide and nitride forming elements, which are Ti, Nb and V. It is a typical strip steel.

2.2. Calculation and its results

The process modelling was carried out for four regimes of deformations that differ by deformation degree and strain rate. Values of the deformation degree and strain rate are given below in table 2.

Table 2

Regimes of deformation

No.	Deformation degree	Strain rate, sec^{-1}
1	0.10	0.5
2	0.10	3.5
3	0.30	0.5
4	0.30	3.5

Deformation temperature, which also was considered as the temperature of precipitation was 950 ºC for all the regimes modelled.

Computation shows that only carbonitrides of Ti and Nb can form at the temperature. Carbides and nitrides of V have significantly lesser temperature of precipitation, so they do not occur under the considered conditions. According to thermodynamic calculations compositions of the carbonitrides formed are as follows: $TiC_{0.58}N_{0.42}$ and $NbC_{0.76}N_{0.24}$.

Primary studied were processes of the particles nucleation and growth. Figure 1 shows increasing of number of the particles by time flowing for Ti and Nb carbonitrides depending on the deformation regime.

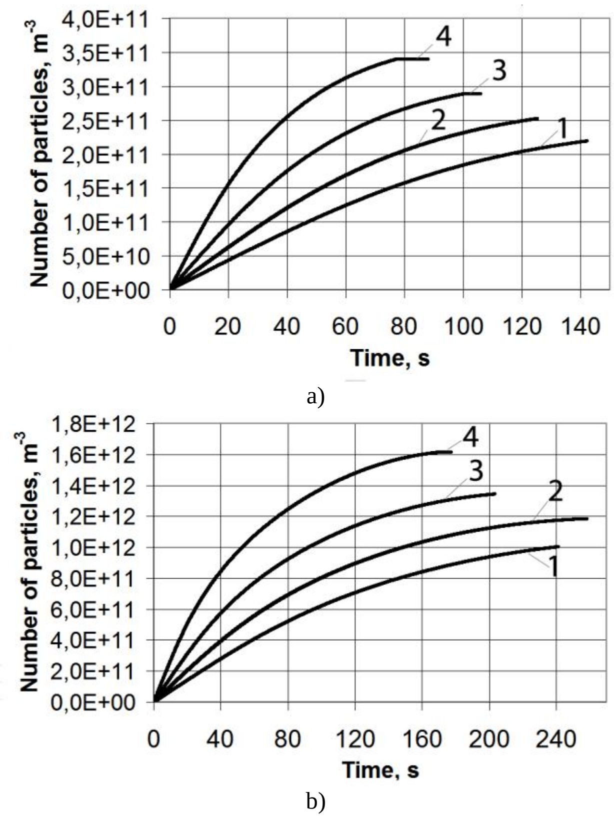


Figure 1 *– Changing by time of number Ti(CN) – (a) and Nb(CN) – (b) particles depending on deformation regime. Numbers near curves correspond to the regimes listed in table 1*

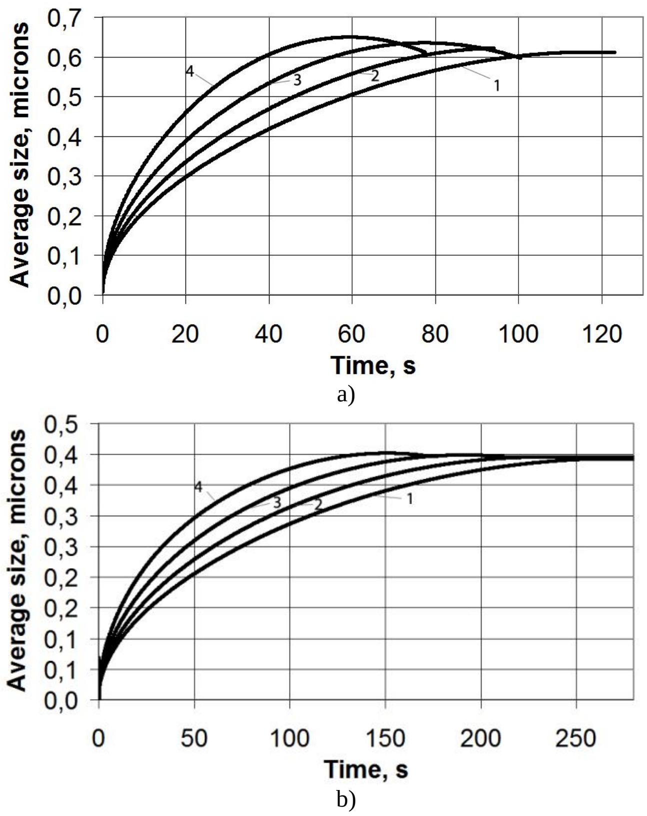


Figure 2 *– Changing by time of average size of Ti(CN) – (a) and Nb(CN) – (b) particles depending on deformation regime. Numbers near curves correspond to the regimes listed in table 1*

Increasing in number of particles occurs owing to nucleation process. When nucleation stops, the increasing stops too. According to the theory accepted in the model, the sites of nucleation of particles are the tersesection sites of dislocations. So increasing of dislocation density during deformation leads to more places of nucleation. Besides increasing of precipitated particles number intensification of deformation also leads to acceleration of nucleation – the process goes faster. Significantly more particles of Nb(CN) precipitate then particles of Ti(CN), which is mostly owing to higher concentration of Nb compeering with Ti in initial chemical composition of the steel. Increasing both of deformation degree and strain rate has significant and similar influence. This distinguishes current situation from that considered in paper [7], where the influence of the strain rate on the kinetics of phase transformations was significantly less than the effect on the deformation degree on it.

In addition to the nucleation process, this model also describes the growth of carbonitride particles. Figure 2 demonstrates changing of the particles average size by the time flowing.

On figure 1 (a) – for Ti(CN) a strange effect is seen. In cases of higher deformation degree, at a certain time the average size of the particles begins to decrease. It is important to note that it's about <u>average</u> size only. Size of each particle grows. This effect is because of new particles nucleation during all the period. The larger a particle is the slower it grows. Intensive deformation makes better conditions for the emergence of a larger number of particles. Hence a situation is possible when originated at an early stage particles are already grown enough to slower their following growth but new ones are keeping appear. This is an explanation of the observed effect of decreasing of average size when all the particles grow. The same effect but significantly lesser is seen for Nb(CN) also that is shown on figure 2 (b).

Another interesting result is that despite the average size growth acceleration intensification of deformation does not affect significantly its final value.

Below in table 3 are given predicted values of final average sizes of the particles obtained at each of the considered deformation regimes.

Table 3

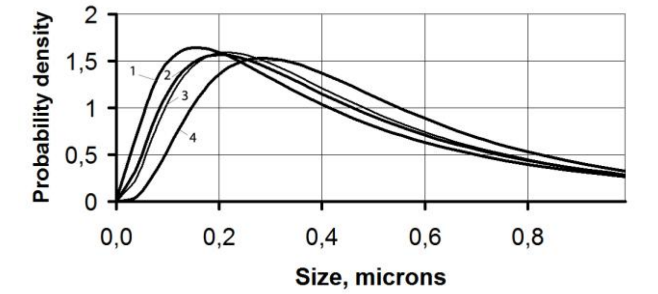
Final average sizes of particles (in nm)

Regime No.	Ti(CN)	Nb(CN)
1	626	401
2	614	397
3	607	391
4	594	382

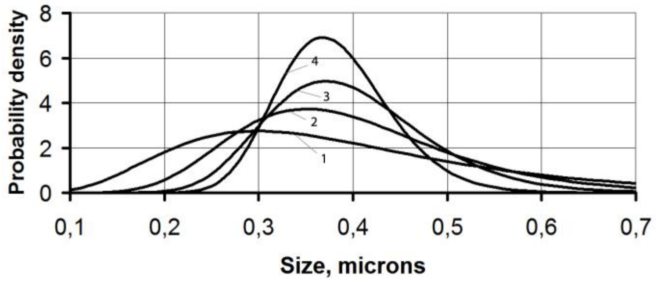
In spite of a little difference in an average size the particles number differs significantly. This effect has the following explanation. Deformation affects more the particle size distribution function then their average size. Plots of the final size distribution density functions predicted using the model are shown on figure 3.

The distribution function is lognormal for all of the cases. More significant influence of deformation regime on size distribution function is observed for Nb(CN) particles. With a lower intensity and degree of deformation, the particle size distribution function looks more smeared. That is, both smaller and larger particles will equally be present in the metal. An increase in the degree and rate of deformation leads to a narrowing of the distribution function and a smaller scatter of medium size. A large role in the narrowing of the distribution function plays an increasing of deformation degree than strain rate, which effect is additional. Deformation effect on distribution function for Ti(CN) particles is lesser but it is also observed. It is noteworthy that in terms of size distribution change for Ti(CN) in this case the effects of strain rate increasing with lower deformation degree is almost to deformation degree magnification but with lesser strain rate.

Thus, the model shows that an increase in the intensity of deformation leads not only to an increase in the number of carbonitride particles, but also narrows the range of variation of their sizes.



a)



b)

Figure 2 *– Final size distribution function of Ti(CN) – (a) and Nb(CN) – (b) particles depending on deformation regime. Numbers near curves correspond to the regimes listed in table 1*

The normal growth of particles at a given temperature stops when the system reaches equilibrium between the carbonitrides and solid solution. That is, simply put, when all that could have precipitate was already precipitated. After that the process of Ostwald ripening begins. It is when particles with smaller size become even smaller and then disappear and larger particles grow taking on material from smaller ones. Ostwald ripening stage of process is also included in the developed model but is out of consideration in current article. It is only to be said that this process is much slower than the nucleation and growth considered above.

3. Conclusions

Using a developed computer model a study was carried out to estimate influence of deformation on kinetics of Ti and Nb carbonitrides precipitation from austenite in low-carbon micro alloyed steel. An influence of the degree and rate of deformation on the number of carbonitride particles, the rate of their nucleation at a temperature of 950 ºC was studied.

Composition of Ti and Nb carbonitrides was predicted for the invalidated conditions, it is $TiC_{0.58}N_{0.42}$ and $NbC_{0.76}N_{0.24}$. Information of chemical composition of carbonitrides is useful to conduct more precise kinetics computation.

It was shown that in spite of small difference in average particles size their amount differs significantly depending on deformation regime. Found here was that degree and rate of deformation affects significantly an obtained size distribution function of the particles precipitated. Especially increasing of both deformation degree and strain rate leads to the dispersion of the distribution becomes smaller.

The obtained results present in the paper are useful for developing of controlled rolling regimes for low-carbon steels micro alloyed with strong carbide and nitride forming elements.

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