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Microstate of Basic Phase of High-Alloyed Ferritic Steels

M.A. Baranov, E.A. Dubov
Altai State Technical University of I.I. Polzunova,
Russian Federation
A Kawałek
Czestochowa University of Technology, **Poland**

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INTRODUCTION

Now ceramics, plastic, carbon-filled-plastic, composites (Mileiko, 1997, Kelly, 1994) gradually trust out metal materials in all spheres of human life. Meanwhile for steels and alloys are not any alternative at manufacturing of critical details of mechanisms and machines testing long sign-variable and shock loads at simultaneous influence of aggressive environment and sharp temperature drops (Shljamnev, 2000, Kositsin,2008). Application criterion of this or that material for manufacturing of given details is conformity of mechanical properties (MP) inherent in it to operation conditions of these details (Fillipov et. al., 2013, Kolokoltsev et al., 2011). The given circumstance transforms MP properties of a material into its consumer properties.

By definition (Guljaev, 1977, Zolotarevskyi, 1983) any of MP is response of material on external mechanical load as plastic deformation. It means that indicators of MP can not be measured by help of the tests admitting only elastic deformations. At the same time they do not yield to calculation by methods of atomic-discrete simulation. The reason of it consists not only in enormous technical and fundamental difficulties of atomic-discrete imitation of testing process of multicomponent, multiphase, macroscopical sample, but also even in successful case of decision of such problem its results could be interpreted no more then correlating with experimental data. Really GOST 1497-84, 9012-59 etc. orders measurement of MP instead of its calculation. In this connection forecasting of MP as expected results of any phenomena can be carried out only by attraction of already available experimental data. However it does not means that forecasting of IMP by atomic-discrete simulation methods appear useless. On the contrary in combination to empirical knowledge and concentration on rather simply calculated parameters correlating with MP indicators could become the effective tool of forecasting. Thus from great variety of factors forming MP indicators it need concentrate only on main of them.

It is necessary to take note that indicators of MP of steel or an alloy are defined by its state – phase and a chemical composition, dispersivity of phases and their distribution on volume of a material. In turn the state of material is formed during its melting and the subsequent thermomechanical treatment (Alexandrov et al., 1982). As opportunities of variation of chemical composition and processing regimes of steels and alloys remain huge then task of MP forecasting as in former times offer interest (Gurkov et al., 1981, Panin,1982).

The solution of above mention problem sees in establishment of correlation between state parameters of basic phase (BP) and indicators of MP on examples of already created materials. As a rule BP represents α or γ solid solution of complex chemical composition on the base of close-paced knot lattice having great number sliding systems (Zhang et al., 2008). Because of the prevailing part binding function and high compliance BP appears the important factor of MP formation for material as a whole.

In spite of fact that just multicomponent disorder phases render the greater influence on MP of a material the binary ordered phases are examined much more narrowly (Shank, 1973, Grinberg & Sjutkina, 1984). Owning to huge number of ways of arrangement of atoms of different sorts atoms on knots of crystal lattice (microstates) the alloys containing big parts of disorder phases are accepted to call as “high entropyed” ones. Last time interest to them steadily grows (Wang et al., 2009, Kuznetsov et al., 2013, Otto et al., 2013).

Any distortions of a crystal lattice of BP certainly are obstacles for dislocation sliding and hence for process of plastic deformation not only for BP but also for the material as a whole. If distortion of crystals of “ordered alloys” and pure metals is caused by grain boundaries, fine-dispersed inclusions cold working deformation then crystals of the disorder solid solutions except of above enumerated factors are deformed owing to displacements of equilibrium positions of atoms concerning knots of perfect lattice. These displacements in turn are caused by an asymmetrical local environment of each of atom. Insignificant on size but distributed on volume of all crystal these distortions essentially reduce mobility of dislocations. In distinguish from cold working deformation they do not disappear at heating of BP down to temperature of its disintegration which is possible coincides with fusion temperature. Just the complex chemical composition of BP instead of dislocation density – the most probable reason of MP stability of highly alloyed steels even after their unprovided heating. The given circumstance is one of reasons that for manufacturing the details testing sharp differences of temperatures (engine valves, disk saws, vanes of steam and gas turbines etc.) are applied high-alloyed steels.

As microstate of BP we shall understand set of coordinates and sorts of atoms forming its crystal lattice. However so detailed information hardly appears useful for explanation of formation of MP indicators. Therefore as macroparameters of BP state it is meaningful to consider the average values of its microstate parameters. Those are certainly the concentration of chemical elements contained in BP. If to exclude from consideration cold working deformation of

material disappearing at heating of material then BP state will be defined only by its chemical composition which owing to redistribution of elements between phases can distinguish from composition of material as a whole. In this connection for definition of BP composition it is necessary to attract the empirical data of state diagrams and foresee regime of subsequent heat treatment of a material. On the other hand it is lawful to consider indicators of MP as state parameters not only BP but of material as a whole. As BP influences on material as a whole it is lawful to assume that between calculated macroparameters of BP and MP indicators also there should be correlation or interrelation (Egorova et al., 2012). We shall accept it as working hypothesis. In according with the stated conception the purpose of the present work is the reconstruction of some of innumerable microstates of α phase of ferritic steels, definition of its macroparameters and their subsequent comparison with indicators of MP of industrially let out steels.

SIMULATION TECHNIQUE

As the state of steel or alloy after its normalizing is close to equilibrium it is necessary to proceed from the equilibrium phase diagram in according to which the concentration of the dissolved carbon in α phase does not exceed 0.01 weight %. Exceed carbon from steel composition is spent for formation of carbides. The metal atoms which present in steel are located mainly in knots of α-lattice.

For a reconstruction of microstate of BF was considered the modelling block of crystal in size 17x17x17 of BCC cells. The sorts of metal atoms located in given knots of lattice were defined by help of the random number generator. Carbon atoms chaotically occupied some of octahedron interpositions so that the chemical composition of the block corresponded to the original composition of BP. As internal energy of the modelling block was understood the energy of interaction of atoms from its central area in size 13x13x13 BCC cells with all other atoms. At the initial stage the equilibrium value of lattice parameter a_0 was found from condition of minimum of internal energy of the block and conservation of all metal atoms in knots of perfect lattice. Then the external borders of the block were fixed and atoms of internal area get opportunity to displace from their starting positions in directions of forces acting on them down to achievement of equilibrium state. As parameters of macrostate of BP were considered binding energy E_B as average value per atom from the central part of the block and distortion degree of crystal lattice. As a measure of this distortion was accepted root-mean-square displacement S_m of atoms of the mobile part of the block concerning their starting positions.

$$S_m = \frac{1}{N}\sqrt{\sum_i (\vec{r}_i - \vec{r}_{i0})^2} \quad (1)$$

where:

N – quantity of atoms of internal area of the block;

$\vec{r}_{i0}$ – radius-vector of knot of perfect lattice;

$\vec{r}_i$ – radius-vector of atom in equilibrium position.

Thus to each carbon atom as interstitial impurity was assigned the displacement equal to half of lattice parameter. Then by help of the special program “microscope” the microstate as a result of simulation was projected on a plane close to cube plane. Thus atoms of a different sorts were represented as circles having one or another pattern. Also here were represented displacement vectors of atoms from their starting positions in equilibrium ones. For presentation they were increased in 10 times.

INTERACTION OF ATOMS

The corner-stone of similar model realization is the adequate quantitative description of interactions of atoms. In frameworks of traditionally used empirical approach (Eckstein,1995) the parameters of plausible potential function are found from conditions of conformity of the calculated and experimental characteristics of properties of substances. Square-law growth of quantity of potentials in dependence on quantity of chemical elements in compound of unordered crystal results in necessity of attraction of huge number of experimental data which simply absent. Therefore the empirical approach is applicable only to binary compounds.

Alternative ab-initio approach assumes a reconstruction of a mathematical image of electronic shells on the base of the Schrödinger equation decision (Schrödinger, 1976) or by density functional method (Cohn, 2002). However the problems accompanying to the ab-initio approach exclude an opportunity of its application to multicomponent compounds. The exit from such situation sees in association of advantages of both approaches. In particular at approximation of distribution function of electronic density its parameters can be found directly from properties of unicomponent substances. The important requirement to distribution function is opportunity of exact analytical representation of electrostatic integrals at mutual overlapping of shells. The similar approach is realized in (Baranov, 2014, Baranov, 2017). The electronic density in shells of atoms was subdivided into internal and peripheral components. The internal electrons were assumed so located that on experimentally observably distances they did not render influence on interaction of atoms. The external shells represented by sphere smeared owing to accommodation on each of its differentially-small element of charge dq_1 distributed under Gauss law. The subsequent integration on surface of sphere allows to reproduce distribution function of peripheral electrons:

$$\rho_1(q_1,\alpha_1,R_1,R)=\frac{1}{4(\sqrt{\pi})^3}\cdot\frac{q_1\alpha_1}{R_1 r}\left[exp(-\alpha_1^2(R-R_1)^2)-exp(-\alpha_1^2(R+R_1)^2)\right] \quad (2)$$

where:

q_1 – charge of sphere,

R_1 – its support radius,

α_1 – Gauss distribution parameter having sense of localization degree of charge near the sphere,

R – distance from the centre.

Interaction of atoms 1 and 2 as a whole is reduced to electrostatic interaction of peripheral shells and compensated by them parts of charges of a nucleus (Baranov, 2017).

$$\phi_C(q_1, q_2, \alpha_1, \alpha_2, R_1, R_2, r) = (nucleus\ 1 + shell\ 1) \times (nucleus\ 2 + shell\ 2) =$$
$$= \frac{q_1 q_2}{r} - q_1 q_2 \cdot g(\alpha_1, R_1, r) - q_1 q_2 \cdot g(\alpha_2, R_2, r) + q_1 q_2 \cdot h(\alpha, R_1, R_2, r) \quad (3)$$

where:

r – distance between nucleus;

$$g(\alpha_1, R_1, r) = \frac{1}{2\alpha_1 R_1 r}[\alpha_1(r + R_1)erf(\alpha_1(r + R_1)) - \alpha_1(r - R_1)erf(\alpha_1(r - R_1))]$$
$$+ \frac{1}{2\sqrt{\pi}\alpha_1 R_1 r}[exp(-\alpha_1^2(r + R_1)^2) - exp(-\alpha_1^2(r - R_1)^2)] \quad (4)$$

- exact analytical expression for energy of coulombic interactions between unite charged smeared on sphere 1 and unite point charge;

$$h(\alpha,\ R_1,\ R_2,\ r) = \frac{1}{8\alpha^2 R_1 R_2 r}[(\alpha^2 a^2 + \frac{1}{2}) \cdot erf(\alpha a) - (\alpha^2 b^2 + \frac{1}{2}) \cdot erf(\alpha b)$$
$$-(\alpha^2 c^2 + \frac{1}{2})erf(\alpha c) + (\alpha^2 d^2 + \frac{1}{2})erf(\alpha d)] + \frac{1}{8\sqrt{\pi}\alpha^2 R_1 R_2 r}[\alpha a\, exp(-\alpha^2 a^2)$$
$$-\alpha b \cdot exp(-\alpha^2 b^2) - \alpha c \cdot exp(-\alpha^2 c^2) + \alpha d \cdot exp(-\alpha^2 d^2)] \quad (5)$$

- exact analytical expression for energy of coulombic interactions between two unite charged smeared on spheres 1 and 2 at their mutual overlapping;

$$\alpha = \frac{\alpha_1 \alpha_2}{\sqrt{\alpha_1^2 + \alpha_2^2}} \quad (6)$$

- parameter of “mutual localization” of overlapped spheres;

$$a = r + R_1 + R_2;\ b = r + R_1 - R_2;\ c = r - R_1 + R_2;\ d = r - R_1 - R_2; \quad (7)$$

- algebraic values. It is typical that at the given approach the parameters of distribution functions of become also parameters of interatomic potential that in turn opens an opportunity of reconstruction of interaction potentials for any pairs of atoms (Zolotarevskyi, 1983).

RESULTS AND DISCUSSION

During research the simulation of a microstates of α phase of 15 industrially let out constructional ferritic steels (Zubthenko, 2003) in state after normalizing have been executed. Weight composition of modelling blocks a phases corresponded to average chemical compositions of steels and are given in Table 1.

Values of macroparameters E_B and S_m of α phase of each mark of steel and IMP (σ_{02}, σ_B, δ, HB) are given in Table 2. Equilibrium value of lattice parameter in all samples of α phase varies insignificantly and close to 2.900 Å.

It is visible from consideration of tables that at increase of strength and hardness also the root-mean-square displacement increase though and not monotonously.

Table 1 Weight concentrations of elements in α phase of steels of ferritic class

№	mark	weight %
1	08X	0.01 C; 0.02 Si; 0.40 Mn; 99.57 Fe;
2	20CrMo	0.01 C; 0.30 Si; 0,55 Cr; 0.70 Mn; 97.94 Fe; 0.50 Mo;
3	20CrMoV	0.01 C; 0.30 Si; 0.25 V; 1,10 Cr; 0.75 Mn; 96.99 Fe; 0.60 Mo;
4	35CrMo	0.01 C; 0.27 Si; 1,00 Cr; 0.55 Mn; 97.57 Fe; 0.20 Ni; 0.20 Cu; 0.20 Mo;
5	15Cr1Mo1V	0.01 C; 0.27 Si; 0.20 V; 1,25 Cr; 0.50 Mn; 96.37 Fe; 0.20 Ni; 0.20 Cu; 1.00 Mo;
6	35CrMoV	0.01 C; 0.30 Si; 0.09 V; 1,00 Cr; 0.60 Mn; 97.50 Fe; 0.20 Ni; 0.20 Cu; 0.10 Mo;
7	20Cr12WNiMoV	0.01 C; 0.50 Si; 0.20 V; 11,50 Cr; 0.70 Mn; 84.89 Fe; 0.70 Ni; 0.60 Mo; 0.90 W;
8	7CrMn2WMoV	0.01 C; 0.25 Si; 0.20 V; 1,60 Cr; 2.00 Mn; 94.09 Fe; 0.30 Ni; 0.20 Cu; 0.65 Mo; 0.70 W;
9	20CrNi2Mo	0.01 C; 0.27 Si; 0,50 Cr; 0.65 Mn; 96.32 Fe; 1.80 Ni; 0.20 Cu; 0.25 Mo;
10	3Cr2MoNiV	0.01 C; 0.25 Si; 0.35 V; 2,30 Cr; 0.45 Mn; 94.54 Fe; 1.40 Ni; 0.20 Cu; 0.50 Mo;
11	34CrNi3Mo	0.01 C; 0.27 Si; 0,90 Cr; 0.65 Mn; 94.85 Fe; 3.00 Ni; 0.32 Mo;
12	30Cr2Ni2MoV	0.01 C; 0.27 Si; 0.23 V; 1,80 Cr; 0.45 Mn; 93.94 Fe; 1.60 Ni; 0.20Cu; 0.30 Mo; 1.20 W;
13	38Cr2Ni3Mo	0.01 C; 0.27 Si; 1,30 Cr; 0.65 Mn; 94.42 Fe; 3.00 Ni; 0.35 Mo;
14	20CrMnNiB	0.01 B; 0.01 C; 0.27 Si; 0.05 Ti; 0,90 Cr; 0.85 Mn; 96.71 Fe; 1.00 Ni; 0.20 Cu;
15	55S2	0.01 C; 1.70 Si; 0,20 Cr; 0.75 Mn; 97.04 Fe; 0.20 Ni; 0.10 Cu;

Table 2 Binding energy, root-mean-square displacement and IMP of ferritic steels

N	mark	indicators of mechanical properties				macroparameters	
		σ_{02}	σ_B	δ, %	HB	E_B, $\frac{eV}{at.}$	Sm, Å
1	08X	175	290	33	131	4.290	0.0603
2	20CrMo	245	441	18	189	4.294	0.0998
3	20CrMoV	275	491	16	189	4.296	0.1014
4	35CrMo	315	570	14	187	4.296	0.1014
5	15Cr1Mo1V	405	550	15	191	4.305	0.1070
6	35CrMoV	410	620	12	-	4.287	0.1064
7	20Cr12WNiMoV	500	750	14	269	4.284	0.1109
8	7CrMn2WMoV	550	930	16	291	4.286	0.1077
9	20CrNi2Mo	685	880	11	341	4.295	0.1006
10	3Cr2MoNiV	705	1150	16	313	4.295	0.1126
11	34CrNi3Mo	735	880	12	299	4.288	0.1038
12	30Cr2Ni2MoV	785	930	11	331	4.201	0.1068
13	38Cr2Ni3Mo	835	980	11	284	4.294	0.1037
14	20CrMnNiB	880	1040	17	286	4.296	0.1096
15	55S2	1100	1350	7	262	4.252	0.1153

In many respects it explains by influence of carbides and in particular by lamellar cementid on IMP. S_m in the greater degree correlates with strength. It is visible for example from comparison of steels 3Cr2MoNiV and 34CrNi3Mo.

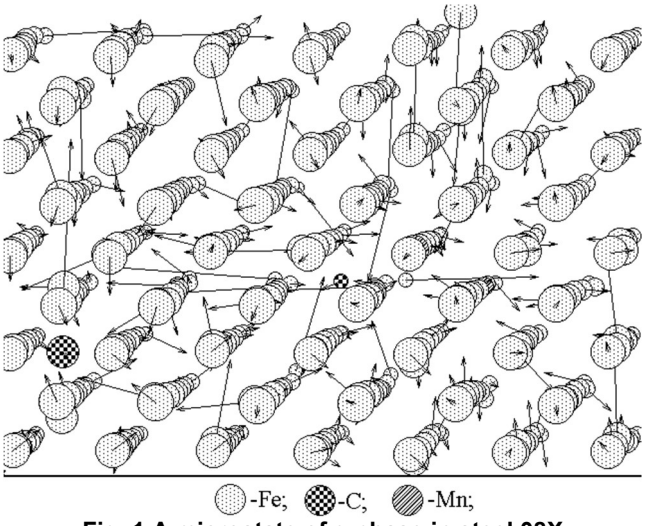

Fig. 1 A microstate of α phase in steel 08X

In Figures 1 and 2 variants of microconditions a phases for steels 08X and 20CrMnNiB are shown.

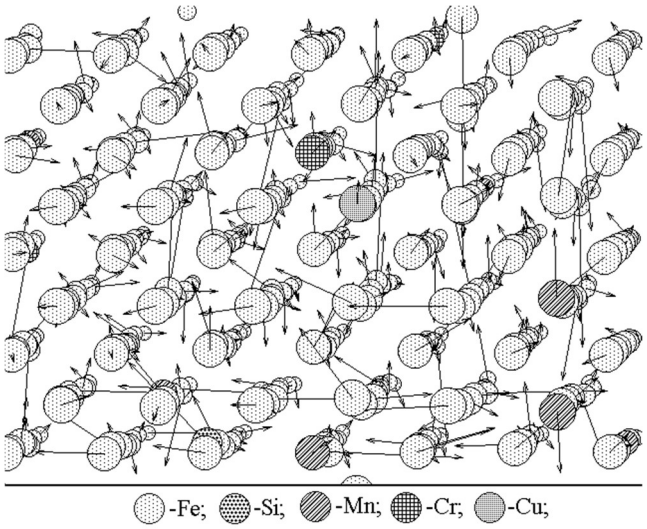

Fig. 2 A microstate of α phase in steel 20CrMnNiB

It is quite expected that in steel 08X there are the tetragonal distortions caused by dissolved carbon. In complex-alloyed steels the greatest distortions are caused by atoms of silicon, manganese, molybdenum and tungsten in positions of substitution impurity.

CONCLUSION

On the example of atomic-discrete simulation of state of concrete steel the efficiency of application of the offered approach combining positive qualities empirical and ab-initio of approaches to description of states of connections of complex chemical compound is proved.

It is natural that within the framework of the offered approach it is impossible to tell anything about corrosion resistance, high temperature stability, casting qualities of a material etc. Its advantage consists in the opportunity of expense less variation of huge quantity of materials of a complex chemical composition with the approached estimation of properties directly connected with a configuration state of BP crystal.

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Abstract.
In according with the stated conception the purpose of the present work is the reconstruction of some of innumerable microstates of α phase of ferritic steels, definition of its macroparameters and their subsequent comparison with indicators of mechanical properties of industrially let out steels. The establishment of a correlation between the measured indicators of mechanical properties of already created materials and the calculated state parameters of their basic phase opens an opportunity of mechanical properties prediction of materials in dependence on their prehistory that as a matter of fact represents the central task of material science. Simulation of α-phase state of series of industrially let out ferritic steels and alloys is executed in the assumption of identity of its composition to composition of steel or alloy as a whole. The correlation between indicators of mechanical properties of steels and alloys and state parameters of their basic phase is traced.

Keywords: high-alloyed ferritic steels, atomic-discrete simulation, crystal lattice of BP