Effect of dynamic blocking of dislocations by interstitial atoms on mechanical properties of metals and alloys

V.V.Shirokov, O.V.Pavlyna, O.V.Shirokov

G.Karpenko Physico-Mechanical Institute, National Academy of Sciences of Ukraine, 5 Naukova St., 79601 Lviv, Ukraine

According to the experimentally approved theoretical calculations it has been established, that under some temperature speed conditions of tension of transition metals and their alloys, a dynamic interaction of the interstitial atoms with dislocations takes place. This effect leads to strengthening of this materils. The temperature of dynamic interaction for hydrogen, oxygen, carbon in iron of two modifications and metals of V-A group are calculated.

Согласно теоретическим расчётам, подтвержденным экспериментально, показано, что при определенных температурно-скоростных условиях растяжения переходных металлов и сплавов на их основе происходит динамическое взаимодейстие атомов внедрения с дислокациями, которое приводит к их упрочнению. Рассчитаны температуры динамического взаимодействия для водорода, азота, кислорода и углерода в железе двух модификаций и металлах V-A группы.

Under certain deformation temperature and rate, the dynamic straining aging (DSA) of metals occurs. It is due to interaction of impurity atoms with freshly formed mobile dislocations being generated during the deforming. This process requires a suitable diffusion mobility of the impurities. Here, the diffusion effect on the loading-induced process is manifested clearly. As a result, within the temperature range of DSA development, the plasticity is decreased and the material hardening occurs.

As the temperature increases, some processes occur favoring the metal or alloy plasticity increase and the strength reduction. The main such processes are the crystal lattice expansion, increase of the atomic vibration amplitude and diffusion mobility of atoms, the coagulation and dissolution of excess structure components, in particular, of the hardening ones, and, as a result, a decrease of the dislocation motion resistance. In general, the dependence of the material strength characteristics, M, on temperature, T, can be described by relationships [1, 2]

$$M = A\exp(Q/RT) \text{ and } M = B\exp(-\beta T)\}, \quad (1)$$

where A, B, β are experimental constants; Q has the sense of the failure process activation energy; R is the gas constant per mole. Basing on Eq.(1), using experimental data on the strength limit σ_b, conditional yield limit $\sigma_{0.2}$, and relative elongation δ, the corresponding plots in $M(T)$, $\lg M(T)$, and $M(1/T)$ can be constructed. In these two cases, the dependences should be approximated by linear sections within the temperature ranges of activity of each hardening mechanism controlling the resistance against plastic deformation of a metal [1, 3]. Experimental dependences evidence, however, that for all materials, nonlinear sections are observed in certain temperature ranges [4−7].

This effect should be explained by the influence of interstitial impurities on properties of metals. This influence is an incontestable fact agreeing with most theoretical concepts of the dislocational origin of the

Table. Calculated DSA temperature intervals for transition metals

Metal	Temperature range, K			
	Carbon	Oxygen	Nitrogen	Hydrogen
V	630...800	640...800	750...940	50...65
Nb	770...970	610...770	790...980	20...30
Ta	890...1130	600...750	890...1125	80...110
Feα	450...560	500...620	390...480	160...195
Feγ	360...460	710...840	755...910	250...320

metal plastic deforming. According to the classification presented in [8], the dislocation interaction conditions with dissolved atoms of foreign elements can be subdivided into three types: (i) mobile dislocations and immobile atoms of dissolved elements, causing the friction resistance of the lattice; (ii) immobile dislocations and mobile atoms of dissolved elements, causing the dislocation blocking by the impurities; and (iii) both the dislocations and the dissolved element atoms are mobile, causing the dynamic straining aging and discontinuous yield under tension. In the course of metal deformation by tension, the interstitial impurities can at certain temperatures form atmospheres (Cottrell atmospheres) that are sufficiently mobile to move together with dislocations [8, 9]. In this case, the metal resistance against ductile deformation (manifesting itself as a hardening) must increase. The calculations presented are valid up to temperatures ≤1000 K. At high temperatures, the similar atmospheres can be formed by interstitial atoms.

Thus, the anomalies in $\sigma_b = f(T)$, $\sigma_{0.2} = f(T)$, $\delta = f(T)$, $\ln\sigma = f(T)$, $\ln\sigma = f(1/T)$ dependences for transition metals can be associated with dynamic interaction of interstitial impurity atoms with dislocations. Since the energy required to tear-off a dislocation from the atmospheres must depend on the saturation of those with impurities, a concentration dependence of the hardening must be expected, no matter what is the method used to introduce the interstitial impurity into the metal. The highest purity vanadium and niobium show the least pronounced anomalies in the property variations.

The true rate of a plastic deformation [6] is

$$\varepsilon' = \Phi \cdot b \cdot L \cdot \upsilon, \qquad (2)$$

where L is the total length of mobile dislocations with the Burgers vector b; υ, the mobile dislocation speed; Φ, the orientation factor. The displacement speed of disloca-

tions surrounded with the impurity atoms is defined by their diffusion [9]:

$$\upsilon = 4D/l, \qquad (3)$$

where D is the impurity diffusion coefficient in the metal; l, the Cottrell atmosphere radius. For mobile dislocations, $L = f \cdot \rho$, where ρ is the dislocation density. Typically, $f = 0.1$; $\Phi = 0.5$; $b = 2.48 \cdot 10^{-8}$ cm; $l = 10 \cdot b$. Basing on (2), (3), we obtain the expression for the deformation rate providing the dislocation interaction with impurity atoms:

$$\dot{\varepsilon} = 2 \cdot 10^{-2} \cdot D \cdot \rho. \qquad (4)$$

Thus, the temperature answering to the maximum influence of an impurity on the strength is individual for each metal and depends on the impurity nature through D. Taking into account the temperature dependence of diffusion coefficient $D = D_0\exp(-Q/RT)$ where Q is the diffusion activation energy; D_0, the pre-exponential factor; R, the gas constant, this temperature is defined as

$$T = Q/R\lg e(-2 + \lg 2 + \lg D_0 - \lg\dot{\varepsilon} + \lg\rho)^{-1}. \qquad (5)$$

Since the relation (5) includes the dislocation density value that depends on the initial state and varies during the loading, the actual active impurity-dislocation interaction occurs within a certain temperature range. The Table presents temperature intervals calculated using (5) for gaseous impurities (O, N, H) and carbon in metals (V, Nb, Fe, Ta) at dislocation density ρ varying from 10^9 to 10^{11} cm^{-2} and the deformation rate $\dot{\varepsilon} = 5 \cdot 10^{-3}$ s^{-1}. Other numerical values in (5) are taken from [10]. It follows from the tabular data that the hydrogen effect at the set deformation rate can be expected at low temperatures (lower than room one), that is confirmed by the results of this work. The temperature intervals for vanadium associated with carbon, oxygen, and
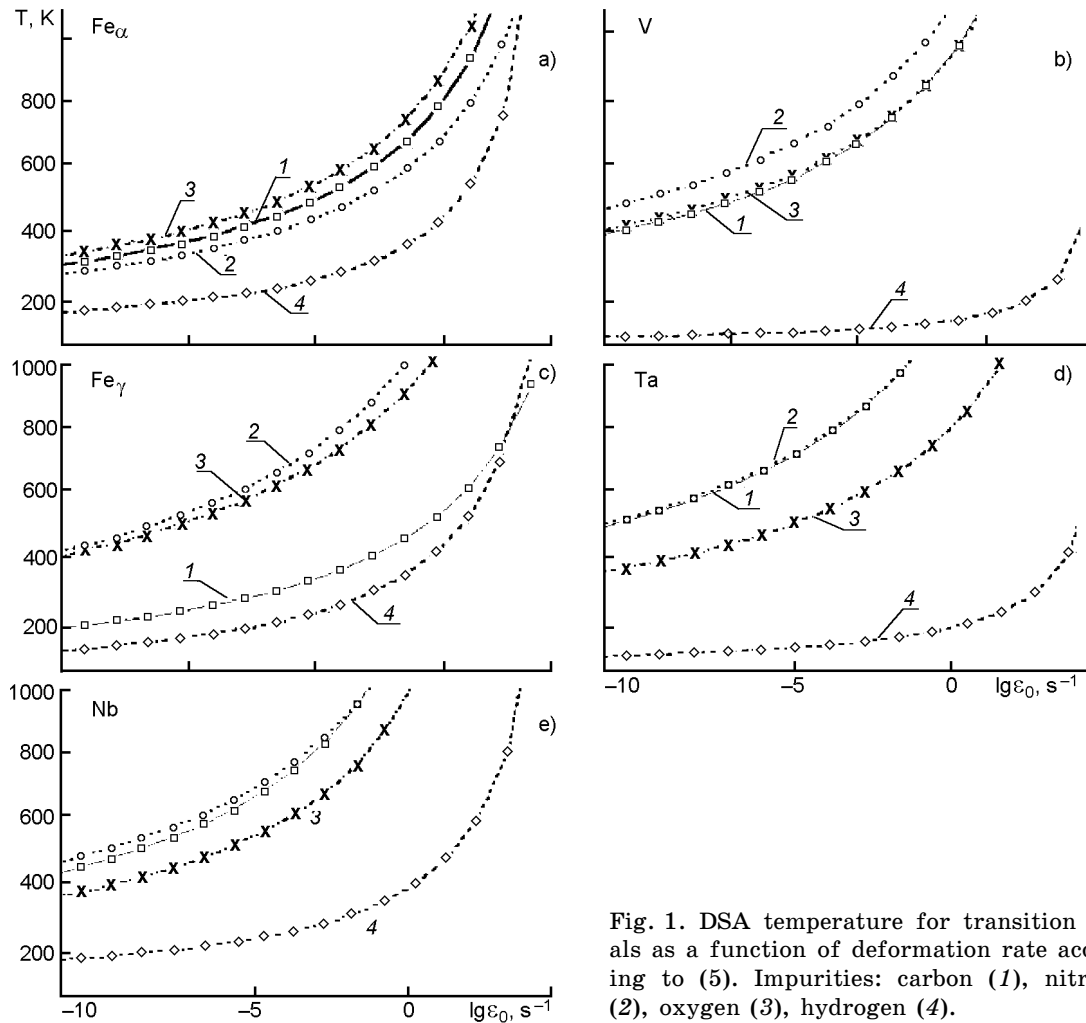
Fig. 1. DSA temperature for transition metals as a function of deformation rate according to (5). Impurities: carbon (*1*), nitrogen (*2*), oxygen (*3*), hydrogen (*4*).

nitrogen are essentially the same, thus, only one anomaly in the temperature dependence of strength is to be expected for this metal. For niobium and tantalum, two temperature intervals are found caused by oxygen and carbon/nitrogen, respectively. As to iron, two temperature intervals for the anomalous plasticity reduction are possible.

The deformation rate is a factor of importance in the impurity atom interaction with dislocations. An increase in the rate can change substantially the DSA temperature interval (Fig. 1), in particular, for hydrogen, thus changing considerably the mechanical behavior of materials in hydrogen-containing atmosphere and under rapid deforming.

Technical purity grade vanadium, niobium, and tantalum were examined in experiments as well as their alloys. The tension strength was measured using a six-position radial type unit [11] in the spectral purity grade argon atmosphere at the deformation rate of $5 \cdot 10^{-3}$ s^{-1}. The examinations

were carried out on annealed specimens and those exposed for 120 h to purified oxygen flow at 1073 K in the unit. To control the gas flow, the 10^{-5} Pa pressure was first provided by oil-free pumping out, then the pressure was increased to 10^{-4} Pa by leaking in technical purity oxygen, and this dynamical flow was maintained during the whole exposure period.

After the 120 h exposure in oxygen atmosphere, the average oxygen concentration (as determined by vacuum melting) was as follows (per cent mass): 0.1 in V; 0.08 in Nb; and 0.06 in Ta samples (in the initial ones, 0.05; 0.01; and 0.04, respectively). Concentrations of other impurities remained unchanged.

Temperature influence on the transition metal strength was examined in wide temperature intervals at 50 K or 273 K steps. The deformation resistance of the metals was determined in different states, namely, in technical purity grade ones, after the
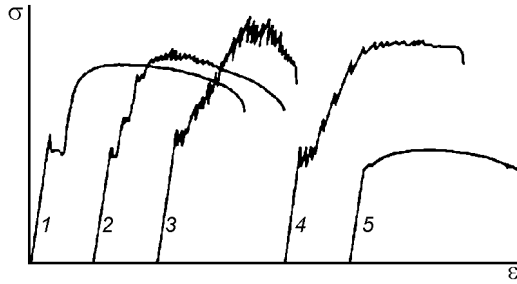
Fig. 2. Tension diagrams of VnM2 alloy at different temperatures. *1* – 293 K, *2* – 573 K, *3* – 673 K, *4* – 773 K, *5* – 1273 K.

standard (recrystallization) heat treatment, and after exposure to oxygen (Fig. 2).

In temperature dependences of mechanical properties for technical purity vanadium (VnM2 grade), a maximum for the strength limit and a minimum for relative elongation have been found. Within the temperature interval 500–700 K, the strength limit is anomalously increased and the yield peak height rises (Fig. 2). Above 700 K, the metal strength drops dramatically as temperature increases under simultaneous plasticization (the relative elongation increases from 25 % at 673 K up to 70–75 % within the 1073–1373 range). In the temperature interval 500–800 K, the tension curves show serration following to the yield plateau; the serration is maximum at 700 K and disappears completely above 800 K. The qualitatively similar regularities in temperature dependences of mechanical properties have been obtained for 45 steel [6], other transition metals, and their alloys.

Exposure to technical purity oxygen flow causes changes in $\sigma_b = f(T)$, $\sigma_{0.2} = f(T)$, $\delta = f(T)$ dependences (Fig. 3). For undoped vanadium the maximum in σ_b rises. The temperature dependences of σ_b and $\sigma_{0.2}$ for niobium and tantalum, two maxima appear at 673 and 873 K as well as the plasticity minima at the same temperatures, thus confirming the DSA temperature interval calculations (see Table).

The Nb–Zr–C alloy characteristics vary in a similar manner (Fig. 3). Note that for all the materials, except for Nb–Zr–C–V–Y system alloy, a discontinuity in the specimen yield has been observed accompanied by serration in tension diagrams. The serration amplitude and frequency depends on the test temperature. The maximum tooth height is observed at temperatures answering to strength peaks. The plastic yield of the Nb–Zr–C–V–Y system alloy is discon-
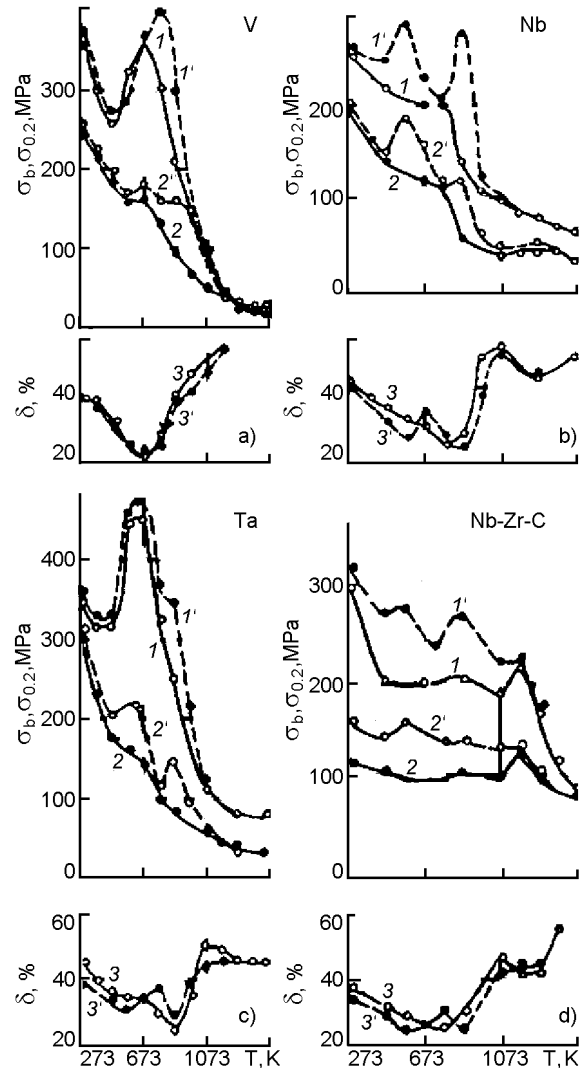

Fig. 3. Temperature dependences of strength limit (*1*, *1'*), yield limit (*2*, *2'*), and relative elongation (*3*, *3'*) of initial metals (*1*, *2*, *3*) and oxygen-enriched ones (*1'*, *2'*, *3'*).

tinuous at above 973 up to 1073 K only. The serration amplitude and frequency are, however, considerably lower than those in tension diagrams obtained at much lower temperatures for other alloys. The exposure in oxygen-containing atmosphere results in an increased serration amplitude at 573 and 873 K but does not influence its frequency above 873 to 973 K.

The appearance of maxima in temperature dependences of strength and yield limits as well as of minima in tension curves above 900 K seems to be related to dislocation interaction with interstitial atoms.

So, in the Nb–Zr–C alloy, the maximum in $\sigma_b = f(T)$, $\sigma_{0.2} = f(T)$ curves at 1073 K may be due to excess zirconium in the solid

solution. The Nb–Zr–C–V–Y system alloy shows also a maximum at 973 K. In this alloy, the interstitial atoms may be in a solid solution, too. In the dependences for a V–Cr binary alloy, there is a pronounced maximum at 1073 K. The absence of a strength increase above 900 K for V–Zr–C alloy is due to a high concentration of interstitial impurities therein. The latter interact with zirconium under formation of a secondary phase, thus excluding it out of the solid solution.

Thus, the interstitial impurities influence considerably the deformability of high-melting metals up to $0.5\,T_m$. The influence temperature range can be subdivided into two ones lying above and under the Cottrell atmosphere formation temperature, respectively. The dislocation blocking occurs in the first range while the de-blocking, in the second one. Comparison of calculated temperature values for deformation rate of 10^{-3} s^{-1} with experimental data shows a satisfactory agreement. It is of importance that within the DSA temperature region, the role of isothermal exposures in dynamic vacuum, helium, lithium and sodium melts increases strongly, as is evidenced by corresponding maxima in temperature dependences of the material mechanical properties. According to calculations, the dynamic interaction of hydrogen with dislocations must occur at temperatures lower than room one, that is confirmed in experiment [7].

References

1. V.A.Borisenko, Hardness and Strength of High-Melting Metals at High Temperatures, Naukova Dumka, Kiev (1984) [in Russian].
2. M.V.Zakharov, L.M.Zakharov, Heat-Resistant Alloys, Metallurgia, Moscow (1972) [in Russian].
3. V.I.Trefilov, Yu.V.Milman, S.A.Firstov, Physical Principles of High-Melting Metal Strength, Naukova Dumka, Kiev (1975) [in Russian].
4. V.V.Shirokov, O.I.Eliseeva, *Fiz.-Khim. Mekhan. Mater.*, No.6, 16 (1982).
5. V.V.Shirokov, Abstr. of Dr. Sci. Thesis, Lviv (1996) [in Ukrainian].
6. V.K.Babich, Yu.P.Gul, I.E.Dolzhenkov, Strain Aging of Steel, Metallurgia, Moscow (1972) [in Russian].
7. K.V.Popov, B.P.Negay, in: Properties and Applications of Heat-Resistant Alloys, Nauka, Moscow (1966), p.218 [in Russian].
8. P.A.Flinn, in: Hardening Mechanisms of Solids, Metallurgia, Moscow (1965), p.25 [in Russian].
9. A.H.Cottrell, Dislocations and Plastic Flow in Crystals, Clarendom Press, Oxford, 1953.
10. E. Fromm, E. Gebhardt, Gase und Kohlenstoff in Metallen, Spinger-Verlag, Berlin Heidelberg New York 1976
11. V.V.Shirokov, O.V.Pavlyna, *Fiz.-Khim. Mekhan. Mater.*, No.5, 106 (2000).

Вплив динамічної взаємодії дислокацій з атомами упровадження на механічні властивості металів та сплавів.

В.В.Широков, О.В.Павлина, О.В.Широков

Згідно теоретичних розрахунків, підтверджених експериментально, показано, що за певних температурно-швидкісних умов розтягування перехідних металів і сплавів на їх основі відбувається динамічна взаємодія атомів упровадження з дислокаціями, яке призводить до їх зміцнення. Розраховано температури динамічної взаємодії для водню, азоту, кисню, і вуглецю в залізі двох модифікацій і металах V-A групи.