

FOREIGN TECHNOLOGY DIVISION



DISTORTION OF THE CRYSTALLINE STRUCTURE AND DENSITY
OF THE DISLOCATIONS IN MOLYBDENUM IN VARIOUS STAGES
OF REFINEMENT AFTER FILING

by

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ABSTRACT The results of the computation of n and ρ are presented Table 3. The mean-statistical number of dislocations n in the accumulation in industrial molybdenum amounts $n = 4.7$, for the alloy Mo+0.1% La, it is equal to $n = 2.7$, whereas for the refined molybdenum $n = 1$. Such an order of change in the value of n in the different specimens of molybdenum fully agrees with the change in its purity and plasticity (Table 1). The lower the purity and plasticity of the molybdenum, the greater the number of dislocations in the accumulation will be. The density of the dislocations in all the cases lies within the limits $10^{11} - 10^{12} \text{ cm}^{-2}$, which corresponds with its typical value for metals in the cold-hardened state. The greater density of the dislocations in the refined molybdenum as compared with industrial molybdenum as compared with industrial molybdenum and the alloy Mo+0.1% La is brought about by the greater plastic deformations in the filing. A comparative evaluation of the levels $\rho_{\Delta a/a}$ and ρ_D enables one to draw an unambiguous conclusion relative to the different character of the interaction and distribution of the dislocations in molybdenum of different purity. English Translation: 9 pages.

The sub delta/a and rho sub D.

10 to the 11th power - 10 to the 12th power / sq cm

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As is known, industrial molybdenum is brittle at room temperature due to the presence of admixtures of inclusions. The explanation of the physical nature of the influence of admixtures on the plasticity of molybdenum is of great scientific interest. In this work a study is made of the distortions of the structure brought about by deformations and the distribution of dislocations in molybdenum of varying purity.

Molybdenum of various purity was obtained through deoxidation by small additions of lanthanum and electron-beam band vacuum fusion (1, 2). The content of oxygen in the molybdenum and the mechanical properties of molybdenum of various purities are given in Table 1.

The specimens for the X-ray analysis were prepared by the filing of slabs. The powder was passed through sieve with a 300 mesh.

For evaluating the distortions of the structure there was used the effect of the expansion of the interference maxima of the metals in the deformation in connection with the pulverization of the crystals and the residual microdeformations. The interference spectra were obtained from copper K_{α} -radiation by means of automatic

Table 1

Mechanical Properties of Molybdenum of Varying Purity

Specimen	Content of oxygen, %	Hardness HV, kG/mm ²	Temperature of transition to brittle state in bending test, °C
Industrial molybdenum . .	0.023*	175	550 (1)
Molybdenum with 0.1% of La	0.002*	157	25 (1)
Refined molybdenum . .	10 ^{-4**}	160	-193 (2)

* The content of oxygen was determined by the method of vacuum fusion.

** The content of oxygen was evaluated by the method of measuring the electrical resistance at 20 and -193° in the laboratory of N. Ye. Alekseyevskiy.

recording on the spectrometer URS-50I. The width of the line was found by means of dividing the area of the maxima of intensity by their height (precision of the measurement of the width, 5%), after which there were introduced corrections for $K \alpha_1 \alpha_2$ and for instrument expansion of the lines with the taking into account of the form of the profiles of the reflexes (3). The separation of the factors of dispersion and the microdeformation, which have an influence on the expansion of the lines were done in accordance with two orders of reflection from the plane (110) for avoiding the errors as a result of the possible anisotropic expansion of the diffractions in accordance with different crystallographic directions (4).

In Table 2 there are shown the values of the true width of the reflexes (110), (220), and there are indicated the portions of the expansion through the pulverization M and the microdeformation N, and also the dimensions of the areas computed on the basis of these data, i. e., the areas of coherent dispersion (a. c. d.) (o. k. p in Russian) and their relative microdeformation $\Delta a/a$ in the direction $\langle 110 \rangle$. It is plain that the dimensions of the a. c. d. of industrial molybdenum are about

Table 2

Value of Areas of Coherent Dispersion (a. c. d.) (o. k. p.)¹ of Relative Deformation $\Delta a/a$ in Molybdenum of Varying Purity

Specimen	True width of reflexes $\beta \cdot 10^3$, rad		Portion in expansion (220) through		D** .106 cm, in direction $\langle 110 \rangle$	$\Delta a/a^{***} \cdot 10^3$ in direction $\langle 110 \rangle$
	110	120	M* of pulverization a. c. d.	N* of micro deformations		
Industrial molybdenum. . .	6.5	15.2	0.18	0.95	7.8	3.8
Molybdenum with 0.1% of La	7.2	15.5	0.29	0.90	4.7	3.6
Refined molybdenum . . .	8.5	15.0	0.58	0.66	2.5	2.6

¹ Translator's note: (o. k. p. = oblasti kogerentnogo rasseyaniya, i. e., areas of coherent dispersion).

$$* \frac{(M+N)^2}{(M+N)^2 + MN} = 1.$$

$$** D = \frac{\lambda \sec \theta}{M}$$

$$*** \Delta a/a = 1/4 N\beta \text{ ctg } \theta.$$

about three times greater than in the case of the refined molybdenum, and the microdeformation is greater by 1.5 times. The values D and $\Delta a/a$ of $\text{Mo}+0.1\% \text{La}$ have interval values between the values for the industrial and the refined molybdenum. As is seen from Table 1, the values of the distortions of the crystalline structure of molybdenum in pulverization are connected with its purity and plasticity.

From the point of view of the dislocation theory, the distortions of the crystalline structure, which are brought out by the given method are the result of the increase in the density of the dislocations in the deformation. The dislocations form boundaries of the areas of coherent dispersion and bring about inner stresses in the lattice.

Thus the density of the dislocations in the deformed molybdenum can be determined from the dimensions of the areas D and the magnitudes of the microdeformation. A comparison of the densities of the dislocations computed from these two values gives the information about the distribution of the dislocations in the deformed molybdenum, which has greater values for the explanation of the processes which are going on in the dormation.

According to the computation by Williamson and Smallman (5), the dependence of the density of the dislocation on the dimension of the blocks or correct areas of the lattice is expressed by the equation

$$\rho = 3n/D^2,$$

where n - is the number of dislocations for each boundary of the block.

On the basis of the theoretical computation of the expansion of the diffraction line as a result of microdeformation brought about by each spiral dislocation in the cubic body-centered lattice (6), the density of the dislocations is connected with the magnitude $\Delta a/a$ determined from the width of the X-ray reflexes by the control (5)

$$\rho = 58 (\Delta a/a)^2 / b^2 F,$$

where b - is the Burgers vector in accordance with the direction $\langle 111 \rangle$ in the cubic body-centered lattice (for molybdenum $b = 2.71 \cdot 10^{-8}$, cm);

F - is the coefficient of the interaction of the dislocations depending on the distribution of the dislocations.

In the simplest case where the dislocations are at great distances from each other and have little interaction, the coefficient F is equal to unity. Such a distribution of the dislocations can be considered as irregular, i. e., for each boundary of the block there is only one dislocation ($n = 1$). In this situation, the indicated equations can be written in the form

$$\rho_D = 3/D^2 \text{ и } \rho_{\Delta a/a} = 58 \left(\frac{\Delta a}{a} \right)^2 / b^2.$$

The formulas presented with connection to the magnitude of the elastic deformation of the lattice with the density of the dislocations are approximate. A more precise expression for ρ takes into account the logarithmic dependence of the energy of the dislocations on the distance between them (5). However, it turns out, that the logarithmic multiple changes slowly as depends on the value D of the functions. Therefore, for the comparison of the levels of the density of the dislocations $\rho_{\Delta a/a}$ in molybdenum of various purity possessing dimensions of the areas of coherent dispersion of a certain order (see Table 2), it is possible to make use of the indicated approximation formulas. The agreement between magnitudes of the densities ρ_D and $\rho_{\Delta a/a}$ computed from the values D and $\Delta a/a$ make possible the assumption of an irregular distribution of the dislocations (or similar to such in accordance with the character of the interaction). In the case of their nonagreement, it is impossible to disregard the interaction of the dislocations and for the computation of the true density ρ , there is necessary, the evaluation of the coefficients F and n .

The densities of the dislocations in the deformed molybdenum of various purity

Table 3

Computation of the Densities of the Dislocations in Accordance with the Size of the Areas of the Coherent Dispersion and Microdeformations $\Delta a/a$ in Molybdenum of Varying Purity After Filing

Specimen	$\Delta a/a \cdot 10^{-3}$	$\rho_{\Delta a/a}, \text{cm}^{-2}$	$D \cdot 10^{-4}, \text{cm}$	ρ_D, cm^{-2}	$n = \left(\frac{\rho_{\Delta a/a}}{\rho_D} \right)^{1/2}$	$\rho = \sqrt{\rho_{\Delta a/a} \cdot \rho_D} \times 10^{11}, \text{cm}^{-2}$
(1) Технический молибден	3,8	$1,1 \cdot 10^{12}$	7,8	$5 \cdot 10^{10}$	4,7	2,3
(2) Молибден с 0,1% La	3,6	$1 \cdot 10^{12}$	4,7	$1,4 \cdot 10^{11}$	2,7	3,7
(3) Очищенный молибден	2,6	$5 \cdot 10^{11}$	2,5	$4,8 \cdot 10^{11}$	1,0	4,9

KEY: (1) Industrial molybdenum, (2) Molybdenum with 0.1% La, (3) Refined molybdenum.

computed from the data in accordance with the distortion of the crystalline structure are given in Table 3. As is seen in the case of the refined molybdenum, the density of the dislocations ρ_D computed in accordance with the size of the areas of coherent dispersion D corresponds with the value $\rho_{\Delta a/a}$ computed in accordance with the microdeformations. This agreement indicates that the true distribution of the dislocations in a given metal corresponds to the model presented above, i. e., it, in accordance with the interaction of the dislocations is similar to the irregular. But for the industrial molybdenum and the alloy Mo+0.1% La $\rho_{\Delta a/a}$, respectively, it is 22 and 7 times as great as for ρ_D . Such a difference can be explained by the distribution of the dislocations in the polygonized walls, or in the form of accumulations in the surfaces of slipping (5). In the first case, the coefficient n and F in the formulas for the computation of ρ , one uses the values $n > 1$ and $F < 1$. The substitution of the values D and $\Delta a/a$ obtained for the impure molybdenum in the equation connecting these values with the density of the dislocations in the polygonized structure (5) has shown that the equation does not have a solution for

$F < 1$. Actually, the high value of the modulus of elasticity of molybdenum excludes the possibility of polygonization in the process of the plastic deformation at room temperature. Thus the nonagreement of the values ρ_D and $\rho_{\Delta a/a}$ can be attributed only to the formation of accumulation of the dislocations in the planes of slippage.

In accordance with the computation (7), with the accumulation of n dislocations in the plane of slippage, the internal stresses for each dislocation increases about n times, i. e., $F = n > 1$. Thus the number of dislocations n in the accumulation and the true density of the dislocations ρ can be computed from the relationships:

$$\rho = n\rho_D = \rho_{\Delta a/a} / n;$$

$$n = (\rho_{\Delta a/a} / \rho_D)^{1/2};$$

$$\rho = (\rho_{\Delta a/a} \cdot \rho_D)^{1/2}.$$

The results of the computation of n and ρ are presented in Table 3. The mean-statistical number of dislocations n in the accumulation in industrial molybdenum amounts $n = 4.7$, for the alloy Mo+0.1% La, it is equal to $n = 2.7$, whereas for the refined molybdenum $n = 1$. Such an order of change in the value of n in the different specimens of molybdenum fully agrees with the change in its purity and plasticity (Table 1). The lower the purity and plasticity of the molybdenum, the greater the number of dislocations in the accumulation will be. The density of the dislocations in all the cases lies within the limits $10^{11} - 10^{12} \text{ cm}^{-2}$, which corresponds with its typical value for metals in the cold-hardened state. The greater density of the dislocations in the refined molybdenum as compared with industrial molybdenum and the alloy Mo+0.1% La is brought about by the greater plastic deformations in the filing. A comparative evaluation of the levels $\rho_{\Delta a/a}$ and ρ_D enables one to draw an unambiguous conclusion relative to the different character of the interaction and distribution of the dislocations in molybdenum of

different purity.

Starting from these data, it turns out that the distribution of the dislocations in the refined molybdenum as to the character of their interaction is similar to the irregular, and in the industrial Mo and the alloy Mo+0.1% La, the dislocations are located in accumulations, the formation of which is linked up with the growth of the fields of elastic stresses. Such a distribution of the dislocations explains well why molybdenum of varying degrees of purity has varying plasticity. The presence of a great amount of admixtures, in particular, admixtures of imbedding in the industrial molybdenum hinders the movement of the dislocations. As a result of this, there are formed accumulations of dislocations on the planes of slippage, which is accompanied by a concentration of dislocation stresses. The concentrations of stresses brings about the breakdown of the metal in little plastic deformations, and therefore, the industrial molybdenum turns out to be brittle. In the case of the refined molybdenum, the absence to such obstacles to the motion of the dislocation results in a higher degree of plastic deformation before breakdown. In this situation, the refined molybdenum possesses lesser dimensions of the a. c. d. and more uniform distribution of the dislocation stresses after deformation.

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