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CONTRIBUTION OF POINT DEFECTS TO THE TEMPERATURE ANOMALY OF THE YIELD STRESS IN SINGLE CRYSTALS OF THE Ni_3Ge ALLOY

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The temperature dependence of the yield stress τ_* of Ni_3Ge single crystals is studied. The temperature dependence $\tau_*(T)$ in the high-temperature region (above 420 K) is found to be conditioned by thermally activated accumulation of the density of non-screw components of superdislocations. Interaction of point defects with edge dislocations and its effect on the temperature anomaly of the yield stress in Ni_3Ge single crystals are analyzed. The calculated results are found to agree with experimental data.

Key words: *yield stress, thermal hardening, edge superdislocations, point defects, superstructure* $L1_2$.

Single crystals of the Ni_3Ge alloy display a significant temperature anomaly of the yield stress τ_* [1–5]. The characteristics of the flow curves and data on the evolution of dislocation substructures in the course of deformation in Ni_3Ge single crystals with different test temperatures were analyzed in detail in [2–5]. It was found that the dependences $\tau_*(T)$ are nonmonotonic, and the ascending branch has segments with different intensities of thermal hardening. In the low-temperature region (below 420 K), the increase in the yield stress in the Ni_3Ge alloy with increasing temperature is caused by formation of Kear–Wilsdorf barriers on the screw components of dislocations. The mechanism of interaction of edge components with point defects and their influence on the yield stress have not been adequately addressed.

The goal of the present work was to analyze the mechanism of interaction of edge components of superdislocations with point defects and the influence of this interaction on the increase in the yield stress in Ni_3Ge single crystals with increasing temperature (at temperatures above 420 K).

The method of preparing the samples, mechanical tests, and research of the dislocation structure of Ni_3Ge single crystals was described in [2, 4]. For different values of strain ε, Fig. 1a shows the temperature dependences of the yield stress for Ni_3Ge single crystals with the directions of the strain axis [001], $[\bar{1}39]$, $[\bar{4}917]$, $[\bar{2}34]$, and $[\bar{1}11]$. The temperature at which these Ni_3Ge single crystals are tested exerts a significant effect on the dependence $\tau_*(T)$. The ascending branch of the curve $\tau_*(T)$ has certain segments characterized by different intensities of thermal hardening. The point $T \approx 420$ K separates the low-temperature segment from the high-temperature segment (at $T > 420$ K). The second segment displays a temperature anomaly of the yield stress, and the maximum on the dependences $\tau_*(T)$ (peak temperature $T_p \approx 873$ K) depends weakly on orientation of the strain axis (Fig. 1a).

The study of the evolution of the dislocation substructure in strained Ni_3Ge single crystals showed that it corresponds to the random and uniform type of substructures [6]. The basic configurations are the straightline and curved superdislocations, dipoles and dipole configurations, and fragments of dislocations [7] in the form of rows of small-radius loops and narrow dipoles. The temperature dependences of the scalar density of dislocations and the density of straightline dislocations $\rho_{\text{str.dis}}(T)$ for different degrees of strain were studied. The scalar density and the density of straightline dislocations increase with increasing strain and test temperatures in the range $T = 77$–293 K. Moreover, the fraction of straightline dislocations W increases with increasing temperature in the low-temperature

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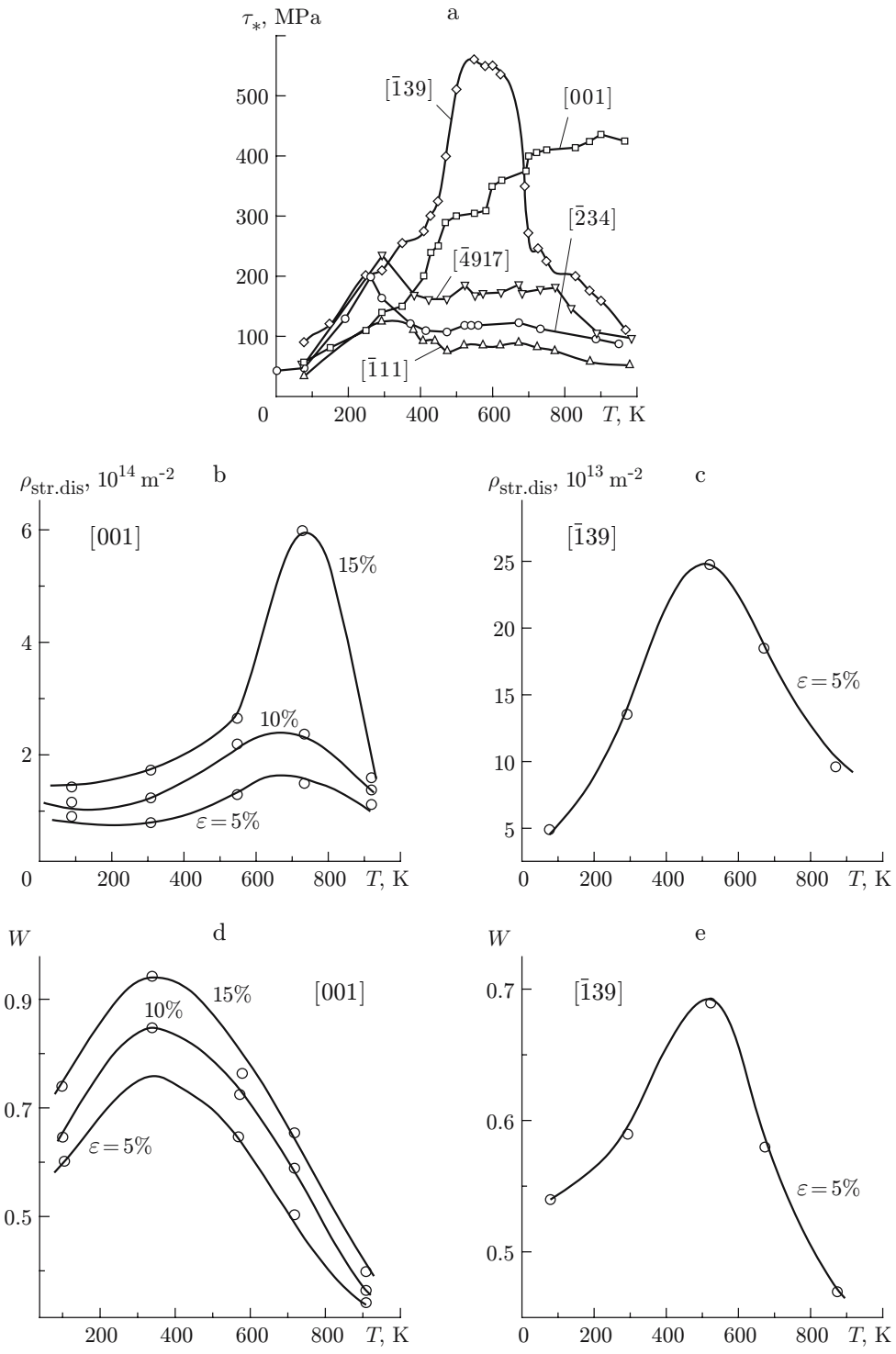

Fig. 1. Yield stress τ_* (a), density of straightline dislocations $\rho_{str.dis}$ (b and c), and fraction of straightline dislocations W (d and e) versus temperature in Ni_3Ge single crystals with different orientations.

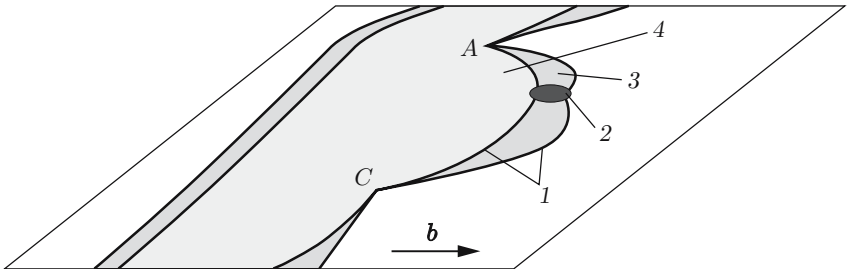

Fig. 2. Interaction of a superpartial dislocation AC with a point defect in the octahedral slip plane (111): 1) superpartial dislocation consisting of two partial Shockley dislocations; 2) deformation point defect; 3) complex stacking fault; 4) antiphase boundary; the points A and C show the locking point of the segment of the superpartial dislocation.

segment (Fig. 1b–e). The fraction W equals the ratio of the density of straightline dislocations to the scalar density. An analysis of the dependence $\tau_*(T)$ (Fig. 1) shows that it correlates with the dependences $\rho_{\text{str.dis}}(T)$ and $W(T)$ in the low-temperature segment. An increase in the dependences $\rho_{\text{str.dis}}(T)$ and $W(T)$ is accompanied by an increase in the dependence $\tau_*(T)$. There are numerous data in publications, which evidence that straightline dislocations are the Kear–Wilsdorf barriers [8–12]. The mobility of screw dislocations decreases with increasing temperature; as a result, the dependence $\rho_{\text{str.dis}}(T)$ increases, and there appear many more Kear–Wilsdorf barriers identified with straightline dislocations in Ni_3Ge single crystals. Abzaev et al. [13] calculated the driving force of formation of the Kear–Wilsdorf barriers on the screw components of superdislocations and estimated their effect on the temperature anomaly $\tau_*(T)$.

It is seen in Figs. 1d and 1e that a significant temperature anomaly of the yield stress in the high-temperature region ($T > 420$ K) of Ni_3Ge single crystals with orientations [001] and $[\bar{1}39]$ is caused by accumulation of dislocations of non-straightline configurations. The temperature growth of the density of non-straightline configurations of superdislocations is caused by interaction of edge components of superdislocations with strain-induced point defects [2–4]. As a result of deposition and trapping of point defects by movable segments of superdislocations, these segments become fixed, and the curved shape is subsequently retained. Up to the peak temperature $T \approx 873$ K, the temperature anomaly $\tau_*(T)$ is conditioned by accumulation of the above-mentioned configurations of superdislocations at the initial stages of deformation. For all these reasons, the temperature dependence of the yield stress corresponding to the ascending branch of $\tau_*(T)$ in single crystals of the Ni_3Ge alloy with different orientations is extremely complicated. The degree of influence of the mechanisms mentioned above depends on the test temperature.

In Ni_3Ge single crystals, deformation proceeds through superdislocations consisting of two superpartial dislocations $a/2\ \langle 110\rangle$ (a is the lattice parameter) connected by an antiphase boundary (APB). The superpartial dislocations are split into the partial Shockley dislocations bound by the complex stacking fault (CSF) with a fairly significant energy (Fig. 2). Indeed, assuming that $\gamma_{\text{CSF}} \approx \gamma_{\text{APB}} + \gamma_{\text{SF}}$, where $\gamma_{\text{APB}} \approx 180$ J/m^2 is the APB energy and $\gamma_{\text{SF}} \approx 100$ J/m^2 is the stacking fault energy, we obtain $\gamma_{\text{CSF}} \approx 280$ J/m^2. Hence, the width of the superpartial dislocation is very small: $r \approx 2$–4 nm [8, 11]. Interaction of edge superdislocations with point defects in Ni_3Ge has some specific features. Single crystals of Ni_3Ge are ordered in accordance with the $L1_2$-type superstructure based on the face-centered cubic packing of atoms, and there is a superstructure organized by hexagonal close packing between the partial Shockley dislocations [12, 14, 15]. The solubilities of point defects in these superstructures are different, which leads to formation of the driving force of the flux of point defects of upward diffusion in the CSF direction.

Figure 2 illustrates the interaction of the edge component of the superdislocation with a point defect in the octahedral slip plane. The point defect locking the dislocation segment is an obstacle of medium strength. Therefore, athermal overcoming of the point defect is little probable. Indeed, superdislocation displacement by the length of the Burgers vector $2b = b + b$ requires stresses $\tau \geqslant [\gamma_{\text{CSF}}/b - (\gamma_{\text{CSF}} - \gamma_{\text{CSF}}(C_{\text{d}}))]$ (C_{d} is the concentration of point defects). For the dislocation to overcome a point obstacle, stresses $\tau \approx \gamma_{\text{CSF}}(C_{\text{d}})/b$ are needed. The presence of a point defect on superpartial dislocations leads to a significant decrease in γ_{CSF} by the value $\gamma_{\text{CSF}}(C_{\text{d}})$,

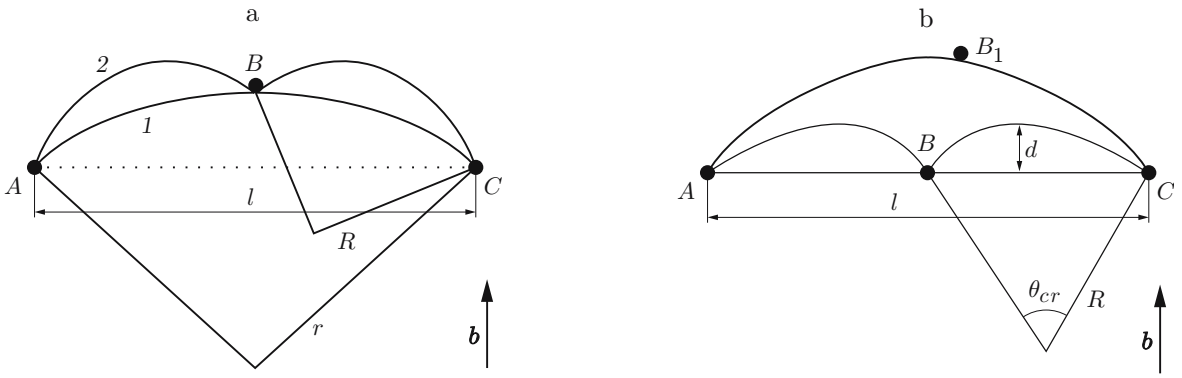

Fig. 3. Interaction of the free segment of a superdislocation AC with a point defect at the point B: (a) locations of the dislocations and point defect; (b) bending of the dislocation segment at the yield stress; the dislocation ABC is shown at the moment of contact with the point defect (1) and at the moment of its separation from the point defect (2).

because γ_{CSF} is a function of the concentration of point defects [16]. For a small width of superpartial dislocations ($r \approx 2$–4 nm), trapping of a point defect (in particular, a vacancy) owing to cleavage of atomic bonds results in a significant change in the energy of the complex stacking fault; hence, $\gamma_{\mathrm{CSF}}(C_{\mathrm{d}})$ becomes a significant fraction of γ_{CSF}. In this case, the stresses $\tau \approx \gamma_{\mathrm{CSF}}(C_{\mathrm{d}})/b$ necessary for the defect to be separated from the dislocation are commensurable with the yield stress at $T_p \approx 873$ K or higher.

Let us consider thermally activated overcoming of a point-defect superdislocation by a free segment. For the Ni_3Ge alloy, a linear dependence between the shear stresses and the scalar density of dislocations is observed for all examined temperatures in the course of deformation [3–5]:

$$\tau = \tau_F + \alpha G b \rho^{1/2}. \tag{1}$$

Here τ_F is the stress of self-locking, α is the parameter of interdislocation interaction, G is the shear modulus, and ρ is the density of dislocations. The left side of Eq. (1) contains external stresses, and the right side of Eq. (1) contains internal stresses: $\tau_{\mathrm{in}} = \tau_F + \alpha G b \rho^{1/2}$ (τ_{in} are internal stresses). Equality (1) shows that the main contribution to internal stresses is made by the linear density of locks on the line of dislocations. The deformation point defects in the slip plane correspond to the locks mentioned. An increase in the yield stress with increasing temperature is largely caused by an increase in the self-locking stresses τ_F due to an increase in temperature [3–5]. The self-locking stress arises owing to formation of the Kear–Wilsdorf barriers on the screw components of superdislocations and interaction of the edge components with point defects. Interaction of the latter results in accumulation of curved configurations of superdislocations at the initial stages of deformation because of the high temperature (see Figs. 1b and 1d).

Equality (1) can be used to find the self-locking stress τ_F induced by interaction of edge dislocations with defects. For two consecutive configurations, the bendings of the free segments ABC (Fig. 3a) interacting with a defect are caused by the stresses $\tau(R)$ and $\tau(r)$. For these segments, the stresses $\tau(R)$ and $\tau(r)$, in accordance with Eq. (1), are related as $W_2/R = \tau_F + W_2/r$ (W_2 is the linear tension of the dislocation). Hence, we have

$$\tau_F = W_2/R - W_2/r \tag{2}$$

(R and r are the bending radii of the dislocation segments).

The points A and C is Fig. 3 are the points of locking by forest dislocations; the points B and B_1 are the neighboring defects in the slip plane. We use Eq. (2) to describe the initial stages of deformation (near the yield stress). In this case, the initial configuration ABC corresponds to the straight line ABC in Fig. 3b. We assume that the point defect is located in the middle of the segment ABC and the self-locking stress τ_F at the yield point equals the stress necessary for the dislocation segment BC to deform to an arc of radius R. The critical angle of bending ($\theta = \theta_{\mathrm{cr}}$) corresponds to separation of the point defect from the dislocation (Fig. 3b). Hence, we obtain

$$\tau_F = W_2/R. \tag{3}$$

The value of τ_F was calculated under the following assumptions. In the slip plane, there is a uniform (random) concentration of deformation point defects. With increasing temperature, the threshold mobility increases and the time needed for separation of the point defect from the dislocation decreases [9, 17]. The concentrations of deformation point defects were calculated in [18]. In particular, the concentration of deformation defects for different test temperatures can be found by the formula

$$\frac{\partial C_{\rm d}}{\partial \gamma} = \frac{p_j \xi B \alpha b \rho^{1/2}}{60}, \tag{4}$$

where p_j is the fraction of threshold-forming forest dislocations, ξ is the fraction of forest dislocations, $B \approx 500$ is the constant determined by the probability of formation of a dislocation compound [18], and γ is the shear. It follows from Eq. (4) that the linear density of defects even at the initial stages of deformation is such that the mean distance between the defects is comparable with the mean distance between the dislocations. Interaction between dislocations and point defects has a non-local character. Such interaction restricts the bending of the free segment AC (Fig. 3b). As is shown in Fig. 3b, the following relation is valid: $d = R(1 - \cos(\theta_{\rm cr}/2))$. Deposition or trapping of the point defect by the dislocation segment at the point B is a random process. A favorable event is an arbitrary part of the dislocation segment AC where defect deposition is possible. Then the formula of the total probability predicts that the probability of the event is $f(AC) = (l/d_1)(d/V)f$, where l is the length of the dislocation segment AC (Fig. 3b), d_1 is the linear size of the defect–dislocation contact region, V is the dislocation velocity, $f = \nu \exp(-U/(kT))$ is the probability of defect jump per unit time, ν is the frequency factor, U is the activation energy of diffusion of the point defect, k is the Boltzmann constant, and T is the temperature. We use the approximation of viscous resistance to bending of the segment AC (Fig. 3b). Then, we obtain $\tau b = BV$. Here $B = 5 \cdot 10^{-4}$ dyn/(sec $\cdot$ cm^2) is the viscosity coefficient [9]; $\sin(\theta_{\rm cr}/2) = l/(2R)$. If the point defect is trapped by the dislocation segment, this event is reliable; hence,

$$\frac{l}{d_1}\,\frac{d}{V}\,f = 1. \tag{5}$$

Using the formulas given above in Eq. (5), we find the radius of bending of the dislocation segment

$$R = \Big(\frac{d_1 W_2}{4\sin(\theta_{\rm cr}/2)(1-\cos(\theta_{\rm cr}/2))Bf}\Big)^{1/3}.$$

Substituting the radius R into Eq. (3), we obtain

$$\tau_F = \frac{2W_2 \sin(\theta_{\rm cr}/2)}{b}\Big(\frac{\cos(\theta_{\rm cr}/2)B\nu}{W_2 d_1}\Big)^{1/3} {\rm e}^{-U/(3kT)}. \tag{6}$$

Assuming the linear tension of the superdislocation to be close to the energy necessary for generating a superdislocation of unit length, we obtain

$$W_2 \approx \gamma_{\rm APB} r - \frac{Gb^2}{2\pi}\,\ln\frac{r}{R_1} + 2Gb^2. \tag{7}$$

Here the first term is the energy of the antiphase boundary, the second term is the energy of interaction of superpartial dislocations, the third term is the intrinsic energy of dislocations, r is the width of the superpartial dislocation, and R_1 is the mean distance between dislocations. Let $G = 8 \cdot 10^4$ MPa, $r \approx 10$ nm, $b \approx 0.25$ nm, $\nu \approx 10^{13}$ sec^{-1}, $\ln(r/R_1) \approx -3$, and $d_1 \approx 0.25$ nm. We substitute these values into Eq. (7). The pre-exponent for these values is approximately $2.05 \cdot 10^4$ MPa.

We approximated the temperature dependences of the yield stress τ_* for Ni_3Ge single crystals with orientations [001] and [$\bar{1}$39]. On the ascending branch of the dependence $\tau_*(T)$ (for $T > 420$ K), the pre-exponents are found to be approximately equal to 10,000 and 46,600 MPa, and the activation energy densities are found to be 3 and 3.3 mJ/m^2 for orientations [001] and [$\bar{1}$39] of Ni_3Ge single crystals, respectively. The activation energy U in Eq. (6) is divided by three. The experimentally obtained activation energy densities equal to 3 and 3.3 mJ/m^2, being divided by three, are close to the density of the activation energy of vacancy migration (about 10 mJ/m^2). A comparison of the numerical values of the pre-exponent in Eq. (7) and experimental results (10,000 and 46,563 MPa, respectively) reveals their good agreement. Because of the non-local character of formation of the Kear-Wilsdorf barriers on the screw components of superdislocations, the driving force of formation of these barriers is also underrated by a factor of three [9–11, 13]. Because of the non-local character of interaction between the

dislocation and the point defect, the effective activation energy is much lower than the energy of migration of point defects. This interaction in the slip plane occurs on an area proportional to the mean distance between dislocations and to the area per one point defect. The activation energies of thermally activated processes determined from the temperature dependences of the yield stress and flow stresses cannot be directly compared with the activation energy of migration of point defects.

Thus, the present study of the temperature dependence of the yield stress allowed us to identify complex nonmonotonic temperature dependences of flow stresses and yield stress. A detailed investigation of dislocation substructures at different test temperatures showed that an increase in τ_* with increasing temperature ($T > 420$ K) is caused by the growth of dislocations of non-straightline configurations. Formation of non-straightline configurations of superdislocations is caused by interaction of these segments with point defects in the octahedral slip plane. This is evidenced by all data of the electron-microscope studies of dislocation substructures at different test temperatures. Allowance for interaction of edge components with point defects with ignored recombination of partial Shockley dislocations makes it possible to describe a significant increase in the yield stress with increasing temperature.

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