Contact formation mechanism between squeezed crystalline solids

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Abstract. The mechanism was proposed and experimentally approved for the final stage of the high temperature contact formation after generation of closed pores in the contact plane. The mechanism is that the pores being healed by the dislocation-diffusion mechanism form assemblages of vacancy type prismatic dislocation loops which alternate with clusters of previously formed interstitial prismatic loops. Between the vacancy-type loops and interstitial ones the diffusion interaction is established resulting in recombination of defects with different signs, the contact formation, pore healing, and decreasing stress and dislocation density in the contact area.

1. Introduction
The problem of interaction of solids in contact and formation of the physical contact is multipronged and actual for modern technologies, namely, fritting, diffusion welding under pressure [1], nano-material preparation [2, 3], as well as under interaction of construction elements in various technology arrangements. The processes in the contact area are multifold and complex, these are determined both by the contacting solids’ properties, and external conditions – temperature, loading, radiation influence, etc. [4-8]. Under conventional conditions, the rate of the contact formation is determined by temperature and loading. Irradiation of construction materials (for example, in nuclear power systems) promotes deformation processes [9, 10] stimulating formation of non-equilibrium point defect concentration, pore generation, and the pore structure evolution, irradiation induced swelling, dynamical recrystallization, dislocation structure evolution, etc. All these factors complicate substantially the processes in the contact area.

Under the contact formation, the solids adjoin by real surfaces which always have roughness of various geometry and scale [11]. Different contact types may be reduced to the extreme case that is the contact of a wedge (roughness) and a plane. That model is usually put into calculations and model experiments on the contact formation investigations.

The model “wedge-plane” allows applying a simple two-dimensional problem of the theory of elasticity for description of stress distribution in the contact plane where the local plastic deformation takes place [12]. It was experimentally shown in [13] that in the early stages, the contact formation process as a result of contortion and embedding the rough edges under certain conditions (high temperature, absence of irradiation, uniaxial compressive loading) occurs by the dislocation-diffusion
mechanism, and its kinetics is controlled by thermal-fluctuation creeping away the dislocation assemblage.

In the present work on the base of the analysis of the contact geometry variations under uniaxial compression of crystalline solids, the substance transfer mechanism was proposed and experimentally approved for the final stage of the process where as a result of contortion and embedding the rough edges, the two-dimensional system of pores is formed.

2. Materials and methods

2.1. Materials and experiment

The experiments were carried out on the samples made from galvanic purified and annealed copper. The samples are shown in figure 1. The sample sizes are 20×10×5 mm.

![Figure 1. Samples for the study](image)

Figure 1. Samples for the study (2α is angle at the wedge vertex, h is the wedge height, W₀ is distance between wedge vertices, W is the contact width).

The rough edges (wedges) were cut on the sample surface and in cross-section looked like triangled jags of \( h = 5 \cdot 10^{-5} \) m height distanced by \( W₀ = 10^{-4} \) m from one another. Annealing under loading was carried out in vacuum 10⁻⁵ mm of mercury at temperature 800°C (0.8\( T_m \)). The width of a formed single contact, as in [12], was measured by the profilometer and averaged not less than by 200 measurements, also, progressively, during experiments by the contact electrical resistivity data.

2.2. Contact geometry evolution during formation and substance transfer mechanism at the final stage

As the contact area expands, the stress distribution changes in the contact area. In the initial time of the contact formation, the loading is given as the force applied per unit length of the sharp wedge (\( P, N/m \)). After the wedge blunting and forming the contact with width \( W \), the loading in the formed contact will be already distributed (\( P/W \)), and further, it will decrease with the contact growing. At that, both the efficiency of dislocation sources and the rate of contact growing caused by dislocation generation and thermo-activated motion are reduced. Direct observations of the dislocation structure evolution [14, 15] under the contact formation between squeezed KCl single crystals in the “wedge-plane” geometry at 0.8 \( T_m \) temperature show that after forming the quasi-stationary dislocation assemblage, the activity of dislocation sources and dislocation density in the contact decrease gradually. The activity of diffusion processes remains unchanged.

In contrast to the model applied in [12, 13] consisted in the system of flat sharp wedges (“comb”) squeezed (crushed) into the plane half-space (figure 1), in the present work, after achieving the contact relative width \( S = W/W₀ \geq 0.5 \) and pore generation, we consider the model of uniaxially compressed plane system of residual voids forming a two-dimensional assemble (figure 2).
Figure 2. The scheme of point defect flows in the final stage of the contact formation (○ – vacancies, ● – interstitial atoms), \( \langle \sigma \rangle = P/W_0 \) is average stress in the contact, P is loading per unit of wedge length.

The problem with voids may be described (to a first approximation assuming the voids independent) using the simple solution of the plane problem for a single void in the uniaxially compressed wide band [16].

From the analysis of the mentioned solution [16] it follows that distribution of shear stress \( \sigma_{xy} \) in Cartesian coordinates XOY with origin in the void center (figure 2) is that in points on the pore surface (for which the polar angle \( \theta = 0^\circ \), \( 180^\circ \) or \( \theta = \pm 90^\circ \) ) \( \sigma_{xy} = \sigma_{yx} = 0 \). For the points with polar angle \( \theta = \pm 45^\circ \) and \( \theta = \pm 135^\circ \) we have \( \sigma_{xy} \equiv (\sigma_{xy})_{\text{max}} \). As the distance from the void center \( x \) increases, these stresses decrease: \( \sigma_{xy} \) is proportional to \( 1/x \) (as in the wedge). The signs «+» and «−» concern to the stress on the right and on the left of the pore. With such stress distribution, under loading, shear dislocation loops [17-19] of different signs may be emitted from the pore surface to different sides of its center (figure 2); the edge components of these loops in total are equivalent to prismatic loops of vacancy type.

The physics of the mechanism proposed for the final stage of the contact formation consists in the following. Under healing by dislocation-diffusion mechanism, assemblages of vacancy-type loops are generated around the pore (figure 2). The vacancy loops and the void undergo as well diffusion dilution caused by their curvature, thus maintaining certain vacancy super-saturation in the neighborhood of the pore. Before the pore formation, the system “wedge-plane” acted efficiently. Each wedge generated interstitial loops. After the pore formation, in the contact plane of the crystal there occur alternating areas occupied by prismatic loops with different signs, i.e. the areas with different dilatation signs alternate. Between these areas, chemical potential gradients occur, resulting in counter-current flows of point defects: vacancies come from healed pores and vacancy loops, and interstitial atoms – from dissolving interstitial loops formed before and generated at present (figure 2). These flows lead to recombination of different sign defects and corresponding dislocation loops, increasing the contact area width \( S \), pore healing, stress relaxation, and decreasing dislocation density at the contact zone. In figure 2 the counter-current flows of opposite sign defects are marked by arrows.

The essential peculiarity of the mechanism under consideration is that unlike the mechanisms discussed in [12, 13] where the substance from the zone of contortion and rough edge embedding was incorporated into surrounding matrix resulting in stress increase and inhibiting the contact formation, in the process described here, due to the counter-current flows, this embedded substance is transferred finally into residual voids. At that, the contact area expands, and the stress created by embedded substance relaxes.

From the described mechanism it is obviously, that its kinetics will be determined by the degree of vacancy super-saturation generated in the crystal lattice by healed pores and vacancy dislocation loops, or other sources connected, for example, with irradiation.
The equation for dilution of an interstitial loop according to the theory [20] is

\[
\frac{dR_1}{dt} = - \frac{2\pi}{b \ln 2R_1/b} \left[ \frac{G \mu (\ln \frac{R_1}{b} + g) D_i \omega}{4\pi(1-v)kT R_1} + D_V \Delta C_V \right]
\]  

(1)

where \( R_1 \) is dislocation loop radius, \( G \) is shear modulus, \( b \) is Burgers vector, \( g \equiv 2 \div 3 \) is value taking into account the energy of the dislocation nucleus, \( D_V, D_l \) are diffusion coefficients for vacancies and interstitials, respectively, at temperature \( T \), \( \omega \) is atomic volume, \( v \) is Poisson coefficient, \( k = 1.38 \cdot 10^{-23} \text{J/K} \) is Boltzmann constant, \( \Delta C_V \) is degree of vacancy super-saturation far from interstitial loops.

In [13] it was established that the observed kinetics of the contact formation is impossible to explain as being limited by dissolution of interstitial loops due to their curvature, that is connected with high activation energy of interstitial generation (4 ± 5 eV for copper).

In the model under consideration, where the plane system of healed pores is assumed, the interstitial loop dissolution takes place due to lattice vacancy supersaturation. Therefore, the first addend in (1) may be neglected, keeping only the second (osmotic) one \( (D_V \Delta C_V) \) in square brackets, so we obtain the kinetics equation for growth of the contact relative width \( S = W/W_0 \), which is controlled by dissolution of interstitial loops. The scheme of such calculation was proposed in [12] and applied in [13]. The essence is in the following. After applying the loading, in the contact, interstitial dislocation loops are emitted and come away at the distance where loading stress is equal to Peierls stress \( \sigma_p \), so the dislocation assemblage is formed.

In the model under consideration, dislocation loop generation is assumed athermic (inhomogeneous). As soon as the difference between external loading stress in the contact and the opposite stress from the dislocation assemblage exceeds the Peierls threshold, \( \sigma_p \), a new dislocation loop is generated. Therefore, the generation rate is not included in the calculation. The process rate is assumed to be controlled by the dislocation loop dissolution rate.

The number of dislocations in the assemblage grows until, after a time, the opposite stress of the assemblage balances the stress from the external loading in the contact. Thus, the dislocation assemblage acquires a quasi-stationary state (with a number of dislocations in the assemblage), to which the contact relative width \( S_{st} \) corresponds. The dislocation assemblage is in dynamical equilibrium. When dislocations go away from the assemblage dissolving by diffusion in the vacancy supersaturation field, new dislocation loops are generated in the contact resulting in its widening. Thus, two flows exist: the flow of interstitial dislocation loop dissolving, and the flow of interstitial dislocation loop generation resulting in the contact expansion. Equating the flows (taking into account the rates of interstitial loop dissolution from (1)) we obtain the equation of the contact growth kinetics in differential form. After its integration taking into account the initial condition (at \( t = t_{st} \), \( S = S_{st} \), where \( S_{st} \) is the contact area at the moment \( t_{st} \), \( t_{st} \) is the formation time of a quasi-stationary dislocation assemblage) we obtain the kinetic equation in integrated form:

\[
S - S_{st} = BD_V \Delta C_V \langle \sigma \rangle (t - t_{st}), \quad B = \frac{4\pi^2(1-v)}{(Gb - 2\pi(1-v)\gamma) b \ln(8R_1/b)}
\]  

(2)

where \( \gamma \) is surface energy density.

The equation (2) is linear by \( \Delta C_V \langle \sigma \rangle \), and \( t \).

3. Results and Discussion

The following dependences were recorded: \( S(t) \) at \( \langle \sigma \rangle \) equal to 2.0\cdot10^7 \text{ N/m}^2, 4.0\cdot10^7 \text{ N/m}^2, 5.0\cdot10^7 \text{ N/m}^2, 7.0\cdot10^7 \text{ N/m}^2; and \( S \langle \sigma \rangle \) at fixed time exposures \( t \) (10, 20, 30, 40, and 50 minutes). In figure 3 a, b, the obtained experimental dependences are shown in accordance with equation (2) as \( (S - S_{st})(t) \) and \( (S - S_{st})(\langle \sigma \rangle) \) (taking into account \( t_{st} \approx 5 \text{ minutes} \) for our experiments). Taking into consideration inaccuracies in \( S \) determination, the relative value of which is about ±(10 ± 15)%, we see that the dependences may be approximated by straight lines.
This allows, using the relation (2), estimating the value $D_{V} \Delta C_{V}$. Taking dispersion into account we obtain the range of values $D_{V} \Delta C_{V} = (10^{-21} \pm 10^{-20})$ m²/s. If to take into consideration that copper self-diffusion coefficient at temperature 800°C is about $D = 4 \cdot 10^{-15}$ m²/s, and vacancy equilibrium concentration is about $2 \cdot 10^{-5}$ at this temperature, then taking into account $D = D_{V} C_{V}$ we obtain the estimation for $\Delta C_{V}$ in the range $10^{-10} \div 10^{-9}$.

On the other hand, it is possible to estimate the vacancy super-saturation degree $\Delta C_{R}$, which occurs in the system due to pore healing and diluting prismatic vacancy loops emitted by pores.

Let us apply the formula from [21]:

$$\Delta C_{R} = \frac{2 \gamma}{R \omega kT} C_{0}. \quad (3)$$

Substituting the values for copper ($\gamma \equiv 0.1 \text{ Gb}$, $G = 4.15 \cdot 10^{10}$ N/m², $b = 3.6 \cdot 10^{-10}$ m, $\omega = 4.7 \cdot 10^{-29}$ m³, and $C_{0} = 2 \cdot 10^{-5}$ for vacancy equilibrium concentration, and $T = 1073$ K experiment temperature) we obtain (taking $R \approx 3 \cdot 10^{-5}$ m): $\Delta C_{R} \approx 3 \cdot 10^{-9}$.

Comparing the estimations of $\Delta C_{V}$ and $\Delta C_{R}$ we see these are of the same order. That allows assuming the proposed physical model of the dislocation-diffusion mechanism for the contact final stage formation consisting in recombination of counter-coming flows of vacancies and interstitials is realistic. The mechanism becomes prevailing as the contact becomes formed and residual pores are generated, because during the process, not only the contact grows, but also stress relaxation between pores takes place in sub-boundary area, and dislocation density decreases due to recombination of dislocation loops of opposite signs.

![Figure 3](image_url)
When the loop size becomes much less than the distance between pores, in the pore assemblage both coalescence and healing takes place which behavior will be determined by temperature and the loading value and character.

4. Conclusion
Analysis of variations of the contact geometry and spatial distribution of mechanical stress in the contact zone during the contact expansion was carried out. It was shown that activity of the dislocation-diffusion mechanism connected with dislocation thermo-fluctuation motion, at the contact relative value \( S = W/W_0 \) more than 0.5 decreases gradually. Along with, the two-dimensional assemble of residual pores forms. The stress field around pores was analyzed, and it was shown that the pores can be healed by dislocation-diffusion mechanism at high temperature. The scheme of the dislocation-diffusion mechanism action was proposed for the contact formation due to recombination of diffusion counter-current flows of point defects: vacancies from pores and vacancy loops, and interstitial atoms – from the interstitial loop assemblages formed before.

Acknowledgment
The authors are sincerely grateful to Dr. of Phys.-Math. Sci., Prof. V.G. Kononenko and to Dr. of Phys.-Math. Sci., Prof. Yu. I. Boyko for the discussion and constructive helpful consults.

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