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Kinetics of setting between dissimilar crystalline materials under thermo deformation effect

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Abstract. It has been established that the kinetic curves of adhesion (strength increase) are of the sigma type with the displacement period of the second stage relative to the first one. The period of this displacement is determined by starting of a marked metal flow over the micro-protrusion contact sections and its passing on the baton into a harder material under the second kind stresses. Activation of the contact surface of a harder material (corundum) occurs due to a handover of the deformation of the surface layer is plastically deformed micro-protrusions (grains) of the metal due to the effect of the second kind of micro-stresses which were much higher minimum yield strength of a harder material, thereby causing plastic deformation of the latter.

1 Introduction

The contact strength is an integral characteristic of the contact interaction of materials in pressure welding at heating. In this case it is obvious that the formation of the physical contact and the activation occur due to plastic deformation of micro-protrusions of a softer metal. Is chosen the temperature of welding below 0.5Tmelt of a harder contact material, for instance sapphire, then due to slow diffusion processes on side of a higher-melting material, the composition of the condensed phase is unchanged, the reaction of this type localized on the interface and the welding process limited only by ″sewing together" of chemical bonds of active atoms of metal and sapphire. Kinetics of adhesion in a contact spot may be contended to show the kinetics of the contact strength increase. The changes of the contact spot cause just on the one hand, a rate change of the contact strength increase with the time and on the other hand, a complex character of micro-kinetics as a whole [1-4].

The central moment is then the phenomenological analysis of the kinetic curves of "sewing together" the bonds according to the regularities of the contact section formation and metal flow over the micro-protrusion contact surface as the base activated factor, and the nature of the activation of the response surface of sapphire being macroplastic unchanged in pressure welding at heating and the thermal activation canal at the temperature below 0.5 T_{melt} of sapphire non-effective [5-10].

A comparison of the kinetic curves of the physical contact formation, plastic deformation of micro-protrusions and contact strength increase (Fig. 1a, b) for a compound Fe50 Ni50 – 60° oriented sapphire show them to be of the sigma type being typical for solid state

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heterogeneous catalysis. From the points of few mentioned above, the development of the contact interaction of different crystal materials at the thermal strain effect is suggested to be explained as follows.

Active atoms with non-compensated bonds move and are supplied to the physical contact surface in smoothing and plastic flow of micro-protrusions metals and out of internal volumes where metal is physically pure. Metal "ruptures" formed on the contact sections of micro-protrusions at plastic flow of metal are active surfaces with non-compensated bonds and decrease their concentration in a closed volume limited by micro-protrusions and sapphire surface in interacting with oxygen atoms.

Depending on these simultaneous processes, the contact sections transform into active surfaces with unsaturated bonds and energetically able to form new chemical bonds with active atoms of another surface (sapphire). Physically sorbed on the responce surface of sapphire, oxygen layers are removed due to the same reasons and mechanical effect of the micro-protrusion metal deformed in their precipitating on sapphire and its dissolution in metal. In other words, metal surfaces of the contact sections are completely purified from adsorbed complex at the first stage of micro-protrusion smoothing and chemically sorbed oxygen layer stays on the surface of sapphire. So, at first two stages of microlug smoothing, no formation of strong bonds of the contact section metal and non-active surface atoms of sapphire occurs. The inhibition of intensive interaction is observed on the kinetic curves of the contact stregnth (adhesion) increase. At this time, a poor interaction between the metal and sapphire is possible as follows: active metal atoms – sapphire chemisorbed oxygen – sapphire. By specimens welded at different process duration corresponding to the first stage of micro-protrusion smoothing, no marked adhesion has been established while "sticking together" has been observed, e.g. poor interaction.

On inhibition, the intensive strength increase of the compound begins (intensive formation of strong chemical bonds) corresponding to the second stage of microprotrusion smoothing. At this time, the relative contact area is more than 0.6 $\overline{S}$nom. The ratio τ/σ of the contact sections reaches a necessary value [11] ensuring the diaplacement of the material point of a contact spot from the axis of symmetry to periphery, e.g. plastic metal flow over the surface of the microprotruslon contact sections is ensured. On the one hand, this fact con firms the activity of metal atoms due to plastic flow, and on the other hand, it promotes the rupture of weakened bonds beween chemisorbed oxygen and sapphire as well as its removal into internal volume of metals. Besides, plastic deformation of the microprotrusion metals due to strain passing on the baton must cause plastic deformation of sapphire or another harder material and its development. On the surface of sapphire plastic deformation traces must be found, for example, bands or slip packs in limits of which active atoms with noncompensated bonds and enegetically able to interact (adhesion) will be formed. Being in a physical contact with the same kind atoms of the response metal surface, such atoms interact and form strong bonds of the mixed type, obviously, due to structural oxygen of sapphire. At this time, the maximum intensity of bond accumulation is observed remaining almost up to the end of plastic flow of the contact section metal. The change of the third stage of microprotrusion smoothing leads to a change of adhesion intensity [12,13].

Thus, both soft and hard materials are plastc deformed in solid contact interacting under presssure at heating of different materials with strong different resistance to plastic deformation and nature of chemical bonds. But their importance in preparing and realization of an elementary adhesion is different. The importance of plastic deformation of metals comes not only to the physical contact formation, activation of the own surface, removal of absorbed oxygen from the surface of a harder material, but also in formation of conditions for occurrance and development of plastic deformation of sapphire. Plastic deformation of a harder material determines its surface activation and development of adhesion. Active surface centres of a harder material (sapphire) occur in points of the microprotrusions formation, e.g.

at the outlet onto the surface of the physical contact zone of bands and slip packs. Depending on the ratio of the stress level at the heaa of dislocation cluster and that of a harder material, only elastic distortions may be occurred in the latter or own bands and slip packs may form in a harder material (sapphire) due to strain passing on the baton on the side of a soft metal. From this moment, the intensity of the contact strength (adhesion) must increase. In other words, starting of the contact strength accumulation will be determined by inhibited development of elastic-plastic deformation of a harder material. Estimate the stress level of the interface metal-sapphire, occurring in a grain of the surface metal layer of the microprotrusion contact sections at deformation in shear and their importance for the development of plastic deformation of sapphire and its surface activation.

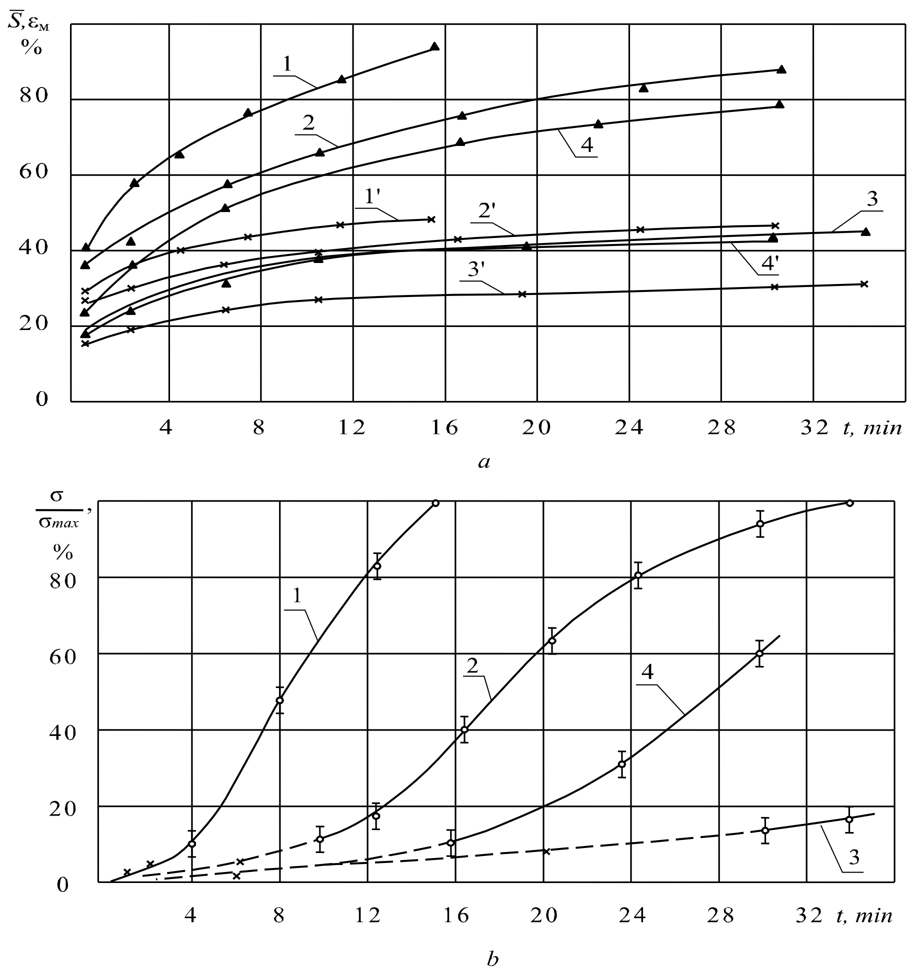


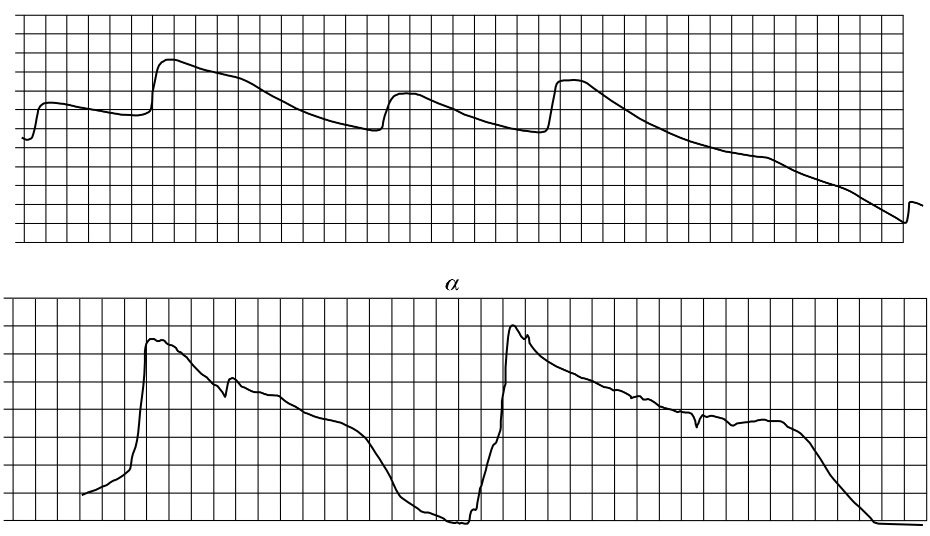
Fig. 1. Kinetics of the physical contact development at the interaction of copper and sapphire (R_z = 40–80 μ). Curves 1, 2, 3 and 4 at σ_n = 80 MPa; 1^1, 2^1, 3^1 and 4^1 at σ_n = 20 MPa. T = 973, 873, 673, 473 K, respectively.

2 The nature of a displacement of adhesion kinetic curve (contact strength increase) for different materials at the thermal strain effect

On the micro-protrusion contact sections, external compression pressure applied causes normal working stresses σ_w which level by the contact interaction decreases discontinuously and approches to a nominal one. Being affected by the contact stresses, a distortion of their side components occurs and metal moves over each contact section from the axis of its symmetry to periphery. A normal stress component σ_w causes a certain contact stress τ_p, of sapphire. It is easily to show that the latter is lower than the punching stresses of sapphire being able to cause its plastic deformation. So, the estimation of the contact stresses caused by the working stresses $\sigma_w = 17.4$ MPa for a pair copper-sapphire at 1173 K and of a moment when the relative area of the physical contact St is as high as 0.6 of the whole area, shows τp of sapphire to be in the range 4.4–8.7 MPa. According to [5,6], the value for a punching stress τ_p (Al_2O_3) of 60° oriented sapphire (e.g. stress components) of the basis plane (0001) and slip direction <1$\bar{1}$20> is equal to 80 MPa, 41 MPa and 20 MPa at 1173 K, 1273 K and 1473 K, respectively.

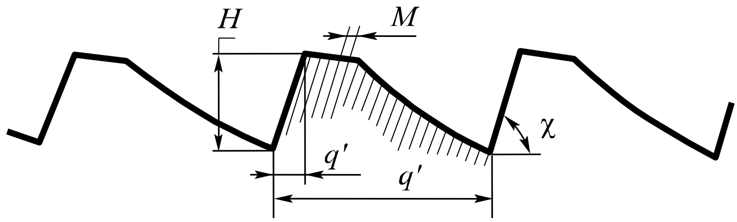
The results of calculations tell that the values of stresses acting on the micro-protrusion contact sections affecting by external pressures don't ensure the level of cleavage stresses τp in sapphire (at least by an order lower) and by themself cannot ensure plastic deformation of sapphire or activation of its surface. In other words, external pressure forms a common background of the stressed state and ensures the physical contact development due to plastic deformation of a "soft" metal.

But the external pressure applied leads to extensive plastic deformation of the surface layer of metals of micro-protrusion contact sections. Besides, plastic deformation traces In form of bands and slip packs ensuring a mirror reflection on the metal surface (Fig. 2a, b) similar to that by welding of different metals [1,3].



a

b



c

Fig. 2. The character of profilograms of the slip pack surface of sapphire (a) by $Fe_{50}Ni_{50}$ (b) and schema of measurements of geometric characteristics of slip packs (c).

Contact stresses occuring in a slip band of the metal surface grain provide the displacement and outlet of dislocations onto the surface of the contact zone where micro-protrusions are formed. In these points, complex strained states are observed. Estimate the contact stresses $\tau_{nc(Me)}$ at the head of dislocation clusters in a slip band of a copper micro-protrusion single grain at the contact with sapphire by the welding mode mentioned above [14-17]. The contact stress at the head of a dislocation cluster of the slip surface of metals with a fee lattice may be determined by the expression

$$\tau_{nc(Me)} = 2d * \frac{\tau^2}{b} * G \tag{1}$$

where: d is grain diameter, τ is shear stress, G is shear modulus, b is Burgers vector. Shear stress τ of copper may be determined

$$\tau = G * \alpha/2p * h \sim G/30 = 1.41 * 10^3\ MPa \tag{2}$$

where: α is lattice parameter, h is interface distance. The value of $\tau_{nc(Me)}$ calculated for copper according to Eq. (1) is $10.6{\cdot}10^3$ MPa. A responce reaction occurs at micro-protrusion formation on the side of sapphire. For geometric reasons, the normal component σ_{Me} of the contact stresses $\tau_{nc(Me)}$ of a slip band of a copper grain is $\sigma_{Me} = \tau_{nc(Me)} \cdot \sin\gamma$, where γ is a "meeting" angle between the slip band of the metal grain and the contact surface of sapphire. Is the "meeting" angle between the micro-protrusion metal grain and sapphire surface equal to 90°, $\tau_{nc(Me)} = \sigma_{Al2O3}$. Usually it must be taken into account the angle Q determining the shear of vector $\tau_{nc(Me)}$ relative to the slip surface. Then the normal component of the slip surface may be determined by the expression

$$\sigma_{Me} = \tau_{nc(Me)} * \sin\gamma * \sin\theta \tag{3}$$

The results of the σ_{Me} calculations for a deforming copper grain depending on the angles γ and θ have given the next values (Table 1).

Table 1. The values for σ_{Me} depending on the "meeting" angle γ and angle θ of the shear vector $\tau_{nc(Me)}$

γ °	θ °	σ_{Me}, MPa
1	1	$2.8 \cdot 10$
1	90	$1.8 \cdot 10^2$
1	45	$1.2 \cdot 10^2$
90	1	$1.8 \cdot 10^2$
45	45	$5.2 \cdot 10^3$
90	45	$7.4 \cdot 10^3$
90	90	$1.06 \cdot 10^4$

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It is evident that the angles γ and θ being, respectively, 1° and 90° are less probable and are to be rejected. By copper with a fee lattice and easy slip in {III}, there is always a family of slip surfaces being at 45° to the contact surface and slip direction. In this case, according to Eq. (3) the value σ_{Me}:

$$\sigma_{Me} = \tau_{nc(Me)} * \sin 45° * \sin 45° = 5.2 * 10^3\ MPa$$

is most probable. The normal component σ_{Me} causes different responce reactions of sapphire σ_{Al2O3}, e.g. $\sigma_{Me} = \sigma_{Al2O3}$. The normal component of sapphire has a contact component $\tau_{p(Al2O3)}$ determined by Shmidt–Boass equation:

$$\tau_{p(Al_2O_3)} = \sigma_{(Al_2O_3)} \cos\varphi * \cos\lambda \tag{4}$$

where: φ is angle between the normal to a slip surface and contracting axis, λ is angle between slip direction and contracting axis.

Estimate probable contact cleavage stresses of sapphire depending on angles φ and λ and normal component of sapphire at the parameters for copper–sapphire welding (Table 2).

Table 2. The values of cleavage stresses of sapphire $\tau_{p(Al_2O_3)}$ depending on the angles φ and λ and normal component $\sigma_{(Al_2O_3)}$

φ°	λ°	σ(Al_2O_3)	τ_p(Al_2O_3)
89	89	28 $5.2·10^3$ $1.06·10^4$	0.0085 1.59 3.24
45	89	28 $5.2·10^3$ $1.06·10^4$	0.34 62.4 $1.27·10^2$
45	45	28 $5.2·10^3$ $1.06·10^4$	13.72 $2.56·10^3$ $5.19·10^3$
45	48	28 $5.2·10^3$ $1.06·10^4$	13.1 $2.43·10^3$ $4.96·10^3$
1	1	28 $5.2·10^3$ $1.06·10^4$	27.44 $5.09·10^3$ $1.03·10^4$
1	45	28 $5.2·10^3$ $1.06·10^4$	19.4 $3.6·10^3$ $7.34·10^3$
1	89	28 $5.2·10^3$ $1.06·10^4$	0.48 88.4 $18·10^2$

Statistics of profilograms made from the surface of sapphire on welding with copper and $Fe_{50}Ni_{50}$ alloy allows one to determine the "meeting" angle φ (45°) between slip bands of sapphire and the contact surface, the angle λ (48°) determined by the x-ray diffraction analysis of sapphire. [5,6,18-21] give the most well-known ratios of φ and λ, as well as Schmidt vectors (74 - 44)° and (22…48)° calculated for φ and λ, respectively; and the product (cos φ ·cos λ) equal to 0.256–0.48. Calculate cleavage stresses of sapphire by (0001) in direction <$1\bar{1}20$> ensuring slight slip at boundary values of Schmidt factor and φ and λ angles. The following values have been calculated:

$\tau_{p(Al2O3)} = (1.33 – 2.49) \cdot 10^3$ MPa.

So, the calculations show that the plastic deformation of the surface layer grains of the micro-protrusion contact sections being affected by external (welding) pressures and stresses of the first kind, causes the formation of micro stresses (stresses of the second kind) in the contact range being some orders higher than the welding stresses of the first kind σ_W. Local stresses of the grain volume cause a res ponce reaction in sapphire leading to plastic deformation of sapphire in form of traces uniform arranged through the nominal section in rough and fine slipping (slip bands and packs) coming onto the surface of the physical contact zone (Table 2).

The formation of slip packs and outlet of slip bands onto the surface of the physical contact zone lead to the formation of deforming "H" high micro-protrusions (Fig. 2b). It has been noted that in welding sapphire with copper, $Fe_{50}Ni_{50}$ alloy and other metals, sapphire sections between slip packs are localized by fine slip lines. In these parts, sapphire is plastic deformed forming micro-protrusions on which adhesion takes place. It is confirmed by comparison of fractograms, profilograms, character of adhesion bridge distribution over the contact sections of micro-protrusions and sapphire.

The calculations of the second kind stresses forming by shear deformation of the grain surface layer of the micro-protrusion contact sections and a comparison of the time necessary to reach the stress level being enough for plastic deformation of sapphire at the moment of an intensive increase of the contact strength show them to be in agreement with the time at which a relative physical contact area is more than 0.6 of the nominal one. The width of single contact sections is then: 0.30–0.32 mm and 0.030–0.032 mm by micro-protrusions of planed surfaces with R_z = 40–80 μ and of burned surfaces with R_z= 3.2–6.3 μ, respectively. Is welding finished, 10–15 slip packs are observed on the surface of sapphire over the whole contour area of the specimen (10 mm diameter). According to [4], sapphire crystals become microplastic at the temperature above 1173 K. At lower temperatures, sapphire is like a brittle substance by compression and bending and is plastic nondeformable. In our experiments on welding, slip packs on sapphire have been observed already at 973 K being, obviously, caused by a sharp expressed stress concentration on the contact sections and microplastic deformation which develops in under-surface layers easylier compared to that in a crystal volume.

The study of the contact surface of sapphire on welding has shown fine slip traces and steps present on the surface. In Table 3, experimental data on the linear size of the step height (H), slip pack width (q,q'), trace number (n) and slip trace distance (M) in a slip pack in welding sapphire with copper and $Fe_{50}Ni_{50}$ alloy depending on the welding temperature and nominal pressure. The experimental results show that at a constant deformation degree of sapphire, the welding temperature and pressure increase causes:

1 – decrease of the micro-protrusion step height of the welded surface of sapphire in slipping;

2 – decrease of the slip pack width, e.g. linear size, under plastic deformation;

3 – increase of the hand number in fine slipping in a pack;

4 – increase of the band density in fine slipping in a pack, e.g. decrease of the distance between working dislocation sources of parallel slip surfaces.

The temperature increase by other things being equal leads to a decrease of the step height "H" and width of slip packs, and an increase of the density of fine slip bans. It has been established the at the constant deformation degree by sapphire, the step is the high the low is the temperature at a constant welding pressure. The displacement increase in rough slip traces at the temperature and pressure decrease is caused by the decrease of these welding parameters affecting the time increase necessary to reach similar total deformation degree of the specimens, e.g. the necessary of rough and fine slipping over the whole cross-section of sapphire. In pressure welding at heating, it means the necessary to increase the process time, e.g. to reach the third and fourth stage of micro-protrusion smoothing [1-4,12].

Assuming the steps at outlet of a band or pack into the zone contacting with the micro-protrusion section in shear deformation of sapphire to he interaction centres where adhesion takes place, estimate linear dimensions of such an activated section for a slip pack, e.g. an average number N of skip packs and band number n in a pack for a single metal grain of the contact section in order to determine the number of shear surfaces at the same time present in a grain. The relationship of an average microscopic rate of the shear deformation γ_{mid} and parameters of the shear deformation of separate grains is described by the expression [22,23]:

$$\gamma_{mid} = N^2 D/d^2(2dt^2b^2)/GkT + Pb^3/kT + (10^{-4}\ e_m)/C_0) \quad (5)$$

where: d is average grain size of the micro-protrusion contact section, D is selfdiffusion coefficient, b is Burger's vector, t is shearing stress, G is shear modulus, K is Boltzmann constant, T is welding temperature, P is sphere tensor of internal stresses, C_O is concentration of the standard state vacancies, e_{ffl} is relative micro-protrusion deformation.

The concentration of the standard state vacancies C_o may be determined according to the expression

$$C_0 = C_v \exp\{-[Gv - (P + p)]\,\Delta V_v/kT) \quad (6)$$

where: C_v is concentration of vacant nodes, G_v is thermodynamical potential of vacancies at zero pressure, P is compression pressure (σ_W in our calculations at the current moment), ΔV_v is volume change at vacancy formation. In welding copper with sapphire at 1173 K and σ_W = 17.4 MPa, it has been calculated the value of $C_o = 4.005 \cdot 10^{18}$ vac/sm^3 [24].

Table 3. Temperature and pressure effect in welding upon the step height H, slip pack width q and q′, traces number n by fine slipping and distance M between traces in a pack on the surface of the micro-protrusion contact sections and sapphire

Contact pair	T, K	σ_n, MPa	H, μ	q, mm	q′, mm	n	M, mm	t_{weld}, s	Relative contact area
Copper + sapphire	973	5	5.8	0.39	0.07	43	0.009	>150	>0.6
	1073	20	3.5	0.34	0.034	52	0.065	>300	>0.7
	1173	20	1.8	0.29	0.032	64	0.0045	>240	>0.7
	973	5	6.0	0.741	0.038	–	–	>150	–
	1073	20	5.3	0.625	0.035	–	–	>300	–
	1173	20	3.8	0.580	0.034	–	–	>240	–
$Fe_{50}Ni_{50}$ alloy + sapphire	1173	5	3.1	0.225	0.024	53	0.0042	>1920	>0.6
	1423	20	2.5	0.151	0.020	66	0.0029	>1440	>0.7
	1473	20	1.8	0.112	0.020	72	0.0015	>960	>0.7
	1173	5	4.3	0.70	0.035	–	–	>1920	–
	1423	20	3.8	0.63	0.037	–	–	>1440	–
	1473	20	3.6	0.60	0.037	–	–	>960	–

Supersaturated concentration of vacancies at the head of a crawling dislocation may be calculated according to the expression

$$C_\tau = C_0 \exp\left[\left(\tau_p + p\right)b^3/KT\right] \quad (7)$$

where: τ_C is contact stresses at the head of dislocation clusters, the other symbols being given in the paper.

In welding copper with sapphire, C_τ has been determined to be $4.05 \cdot 10^{18}$ vac/sm^3. The comparison of C_o and C_τ have shown the sphere stress tensor "p" contribution into vacancy supersaturation to be small. The estimation of the first three members of Eq. (5) has given following values:

$$2dt^2 b^2 / GKT = 1.79 \cdot 10^{-17},\ pb^3/KT = 1.73 \cdot 10^{-4},\quad 10^{-4}e_m / C_o = 0.973.$$

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The calculations show that the main contribution into the rate of the shear deformation is made by the third member, e.g., deformation component. The contribution of the first and second members may be neglected. Eq. (5) is then expressed by

$$\gamma_{mid} = \mathrm{N}^2\mathrm{D} \,/\, d^2 \cdot 0.98 \tag{8}$$

Assuming $\gamma_{mid} = 1.44 \cdot 10^{-3}\ \mathrm{s}^{-1}$ for $d = 3\mu$ according to the experimental results, one obtains $N = 0.59$. In other words, the relative linear size of the activated part of a slip pack is ~ 0.60. Is assumed the distance between slip packs to be 1, and 100% of atoms of the metal grain surface of the contact section or sapphire to be at the physical contact, only 60% of them will be transformed into an active state due to slip pack deformation. The other surface atoms being at the physical contact will be activated due to line slipping characterized by a damped slop of sigma curves of the contact strength increase. This fact is confirmed by the kinetic curves of the contact strength increase.

Estimate now the linear size of the activated part of the micro-protrusion contact section of copper of in slip pack. The product (nq)S determines the size (relative values) of an activated part at the linear size of the single contact section $\overline{\mathrm{S}} = 0.030–0.032$ mm, width of the slip pack q and slip band number n (*Table 4*):

Table 4. Influence of temperature and pressure on the value of the linear size of the activated area

T,K	σ_n, MPa	nq	$(\mathrm{nq})\overline{\mathrm{S}}$
973	5	16.77	0.50
1073	20	17.68	0.53
1173	20	18.56	0.56

A good correlation of calculated and experimental results is to be noted. With increasing temperature and pressure, the strength intensity increases, welding time decreases and linear dimensions of the activated parts of a slip pack near Eq. (5).

3 Conclusion

1. By theory of the development of local plastic deformation, comparison of calculated and experimental results, it has been shown a clear correlation of the density of adhesion centres, slip packs in the near-contact zone of a harder material (on the one hand), deformation degree of micro-protrusions, area of the contact sections and the starting moment of an intensive increase of the contact strength (on the other hand). The mechanical channel of activation of the contact surfaces has been found to be the main one under the conditions discussed above.
2. The external pressure applied ensures the stresses of the first kind which are too small for plastic deformation of a harder material hut they form a common background of the stressed state and ensure the physical contact development due to micro-protrusion smoothing. Shear plastic deformation of the surface layer grains of the contact sections being in the physical contact with a response surface of a harder material cause micro-stresses, which transfer into a harder material leads just to plastic deformation of the latter.

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