PHONON CONCEPTION OF METAL AND ALLOY FRACTURE

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Phonon conception of metal and alloy fracture being developed by the author is represented here in conformity with what the decisive role in fracture belongs to the phonon subsystem of lattice. It is supposed that the presence of dislocations in crystals causes the appearance of specific vibration modes in phonon spectrum. And the superposition of quantum vibrations of these modes results in bonds split in lattice. The experiments carried out support the basic states of the conception.

Nowadays there are numerous proofs of the important role played by phonon subsystem in the fracture process of solids (1-4). On the basis of "phonon theory of brittle fracture" the calculation of surface energy of several metals was made (1,2). It was obtained quite satisfactory agreement between values calculated of surface energy and surface energy values obtained experimenally and from other theoretical preconditions. In the study (3) a conclusion on the basis of fundamental theoretical generalization was drawn that the dislocation systems in crystals are prospective for observation of phonon maser and superradiative effects. As a result the spontaneous appearance of elastic energy pulses of high power is possible resulting in machine parts and units fracture. At last the appearance of local and resonance vibrations in phonon spectrum can cause (4) a considerable change in activation energy of bonds decay.

Recently the author proposed (5) phonon conception of fracture of real metals in conformity with what the

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phonon subsystem plays the decisive role in atomic bonds split in lattice. At the same time the particular influence caused by dislocations on the phonon subsystem is stressed: in local volumes of lattice due to the presence of dislocations the phonon spectrum is cut on the side of minimum wavelength $\lambda_i = 2D_i$, where D_i - is effective width of dislocations core in the corresponding direction of lattice wave propagation. With the increasing of dislocations density, level of internal energy in lattice increases and on reaching critical density of dislocations it reaches the threshold value, equals to $W_i = h s_i / \lambda_i = h\nu_i$, where s_i - sound speed in the corresponding directions of lattice, ν_i - frequency of the corresponding vibration mode, h - Plank's constant. This energy absorption by crystal lattice causes sharp amplitude increasing of atomic vibration of i -mode.

Each metal (and alloys on its base) has its own discrete spectrum of threshold energy levels W_i . Alloying and thermal treatment change this spectrum only in inconsiderable degree (5), however they influence on the position of the main threshold energy level W_i^o, corresponding to the main threshold i_o-mode of vibration. Interatomic bonds split in lattice occurs during superposition of quantum vibration (phonons) of i_o-mode. That is why it can be supposed that for each metal or alloy in this or that structural condition it is characteristic the presence in its lattice of the main vibration mode, responsible for the interatomic bonds split.

The threshold energy levels W_i were calculated for several industrially important metals with different types of lattice: Al, Ti, α-Fe, Ni, Cu,Mo. The width of typical dislocatin cores is determined usually by the methods of molecular dynamics. It's quite labour-intensive process, so the values of the above parameter of dislocations are known only for the limited number of metals. Among them are α-Fe, Cu, Mo. For the rest of the metals investigated the cores dimentions of typical dislocations were calculated in this study. The procedure of obtaining of these characteristics is demonstrated below on example of calculation of width and energy of full edge dislocation $\langle 112 \rangle$ (with vector $a/2)\langle 110 \rangle$, where a - lattice constant) in an F.C.C. metal of Al lattice.

The crystallite investigated contained 975 atoms in one identity period, and pair interatomic interaction was described by Morze potential:

$$U(r_{ij}) = U_0\left(e^{-2\alpha(r_{ij}-r_0)} - 2e^{-\alpha(r_{ij}-r_0)}\right), \qquad (1)$$

Where r_0, U_0, α constants are taken from study (6). The influence of potential during calculation was bounded by 176 neigbour atoms. The calculations were made on computer. Initially the energy of each atom corresponding to ideal lattice was calculated according to formula:

$$U_i = \sum_{j=1}^{176} U(r_{ij}), \qquad (2)$$

where r_{ij} - distance between atoms i, j ; j - number of atoms in the shere of influence. Then the initial configuration of crystallite atoms was constructed, corresponding to the elastic-atomic model of edge dislocation according to the method (7). For the finding of equilibrium configuration of atoms the periodic boundary conditions were superimposed on the external faces of crystallite perpendicular to the dislocation line and the strict boundary conditions were superimposed on the faces parallel to the dislocation line at sufficient distance from the dislocation core. After superimposing boundary conditions for 460 mobile atoms 3x460 classical movement equations at moment t were solved:

$$\ddot{x}_j^i(t) = m^{-1} F_j^i(t) \qquad (3)$$

For solving of equations (3) method of central differences was applied:

$$\dot{x}_j^i(t+\Delta t/2) = \dot{x}_j^i(t-\Delta t/2) + (\Delta t/m)F_j^i(t)$$
$$x_j^i(t+\Delta t) = x_j^i(t) + \Delta t\, \dot{x}_j^i(t+\Delta t)/2 \qquad (4)$$

Here Δt - integration step. For Al $\Delta t = 2{,}389 \cdot 10^{-15}$ sec. The regularity of solution of movement equations at each time step was controlled by the testing of fulfilment in the system of law of energy conservation. After M time steps correlation

$$K(M\Delta t) = U(M\Delta t) - U(0), \qquad (5)$$

where U(M t) - U(0) - work made in the system by forces of interatomic interaction must be fulfilled accurate not less than $1{,}602 \cdot 10^{-24}$ j. The solving of equations was being made until kinetic energy of the system reduced below $1{,}602 \cdot 10^{-24}$ j. For reducing of calculation time the additional procedure of artificial energy dissipation was used. The energy of dislocation simulated was calculated as function of distance from the dislo-

cation center and within limits of radius being determined it was calculated according to formula:

$$U = \frac{1}{2} \sum_{i=1}^{n} (U_i - U_0), \qquad (6)$$

where n - number of atoms inside sphere, bounded by this radius, U_i - energy of i - atom after relaxation, U_0 - energy of atom in ideal crystal. Then the dependence graph of edge dislocation energy on distance logarithm to the dislocation line was made. The linear portion on the graph determined the field of application of continual theory. That r, at what the linear dependence violated, was considered to be the radius of dislocation core r_c. The calculations given showed that in Al lattice core radius of the full boundary dislocation considered $r_c = 3{,}6\ d_0$ (d_0 - distance between the nearest neighbour atoms), then $D_c = 7{,}2\ d_0$. The dimentions of dislocation core were determined not only in the direction for example of $[\bar{1}01]$ ($D_c = D_{\bar{1}01}$), but also in other possible directions of lattice wave propagation $[0\bar{1}1]$ and $[\bar{1}10]$: $D_{0\bar{1}1} = D_{\bar{1}10} = 14{,}4\ d_0$.

For the full screw dislocation in Al lattice situated for example in plane (111) along direction $[\bar{1}01]$ the calculations according to the method described above gave following values of the effective dislocation width: $D_c = D_{\bar{1}2\bar{1}} = 4{,}2\ d_0$, $D_{0\bar{1}1} = D_{\bar{1}10} = 4{,}85\ d_0$.

Similarly values D_i were estimated for typical dislocations in other metals. The levels of energy W_i were calculated using the table values of propagation speed of longitudinal and cross waves in the corresponding directions of lattice.

The testing of regularity of the conception being developed was carried out in two directions. First of all it was necessary to be assured of the presence of descrete spectrum of threshold levels of energy W_i for each metal and alloys on its base. For this purpose the upsetting of cylindrical specimens on the vertical impact machine was made. The energy supplied was determined as the product of load weight into lift height. With this energy being referred to the specimen volume we obtained the value of specific mechanical energy A supplied. Before and after the upsetting specimens the wide complex of physical-mechanical properties was determined: residual deformation, temperature, microhardness, fine structure parameters. Data on the above characteristcs change were shown graphically in dependence on specific energy A supplied. It was determined that the sharp change of material properties falls just on

those deformation regimes at what value A becomes equwal to threshold values W_i calculated for the material given. The examples of such properties change are shown on Figure 1, where vertical lines show spectrum of values W_i (designated in order of increase as $W_\alpha, W_\beta, W_\gamma, W_\delta, W_\varepsilon$). According to Figure 1 at $A = W_i$ the intensity of deformation growth sharply slows down and even becomes negative. It is interesting to note, that the above effect is observed when energy supplied is a multiple of W_i, i.e. at $A = nW_i$, where n = 1, 2, 3,..

If to consider that the maximum value of the latent energy of cold hardening U_ζ^{max} corresponds to the main level of energy W_i^0 for the metal or alloy given, then the testing of regularity of the model proposed can be carried out by another way. As it was shown earlier (8), U_ζ^{max} is close to the value of full work of uniform deformation A_e, which in its turn can be expressed through the known material mechanical characteristics. It facilitates considerably the solving of the problem raised: it's sufficient to determine values A_e for alloys and to compare them with threshold values of energy W_i, calculated for alloys base. In study (5) such comparison was made for steels and Al alloys. On Figure 2 data for Ti alloys are given. In all cases values A_e of alloys are close to one of the threshold values of energy W_i ($A_e = W_i^0$), calculated on constant data of pure metals.

With base diagrams similar to that shown on Figure 2 for every type of alloys it is possible to carry out the purposeful choise of materials with optimal structure, providing maximum power consumption at fracture loading.

REFERENCES

(1) Caglioti,G., Rizzi,G., Bilello,J.C.,J.Appl. Phys.,Vol.42,No.11,1971,pp.4271-4276.

(2) Caglioti,G., Rizzi,G., Bilello,J.C.,J.Appl. Phys.,Vol.43,No.8,1972,pp.3600-3601.

(3) Alekseev,A.V., Kopvillem,U.Kh.,Ukrainian J. Phys.,No.23,1978,pp.1194-1205.

(4) Bartenev,G.M., Savin,E.S.,High mol.comp., Vol.23,No.12,1981,pp.2757-2764.

(5) Ragozin,Yu.I.,Proc.of the 7th European conf. on fracture,Budapest,H.,Vol.1,1978,pp.109-111.

(6) Kenzhaev,K., Shemyi-Zade,V.E., "Parameters of Morze potential of 25 metals of cubic symmetry", Institute of metals physics, SD AS USSR, Tomsk, 1978, 5p., Dep.in VINITI, 12.01.78, No.395-78D.

(7) Plishkin,Yu.M., Sikhin,S.N., "Calculation of dislocation core structure in cubic crystals by simulation method", Institute of metals physics, USC AS USSR, Sverdlovsk, 1976, 43p., Dep.in VINITI, 01.09.76, No.3291-76D.

(8) Ragozin,Yu.I., Antonov,Yu.Ya., Problemy Prochnosty, No.2, 1984, pp.28-32.

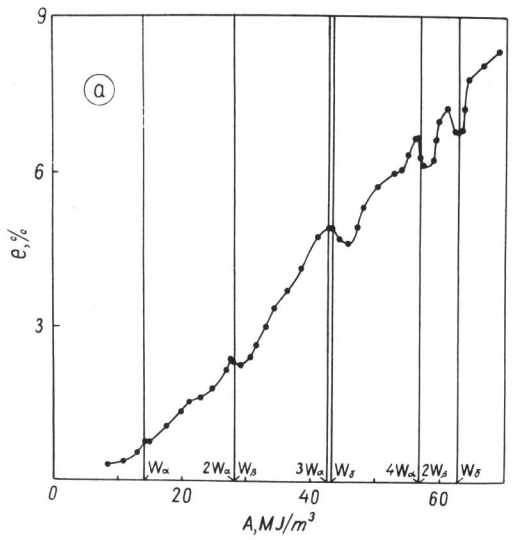

Figure 1 Dependence of true deformation e of cylinder specimens on value of specific energy A supplied at impact upsetting; *a* - alloy AK8; *б* - alloy VT3-1.

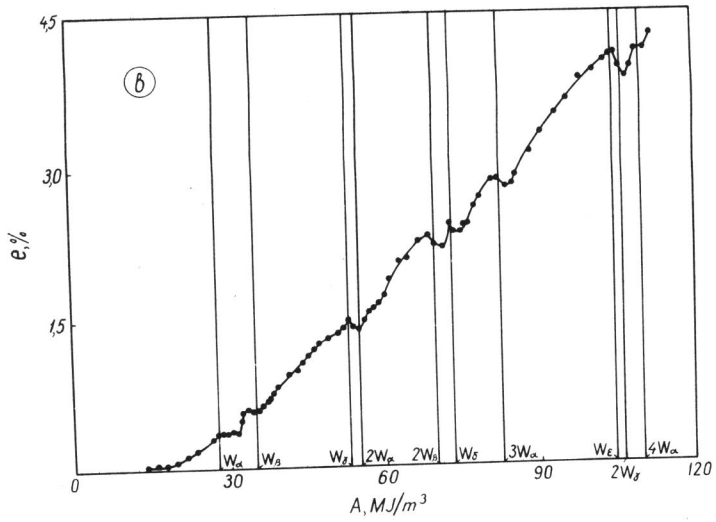

Figure 1 (Cont.)

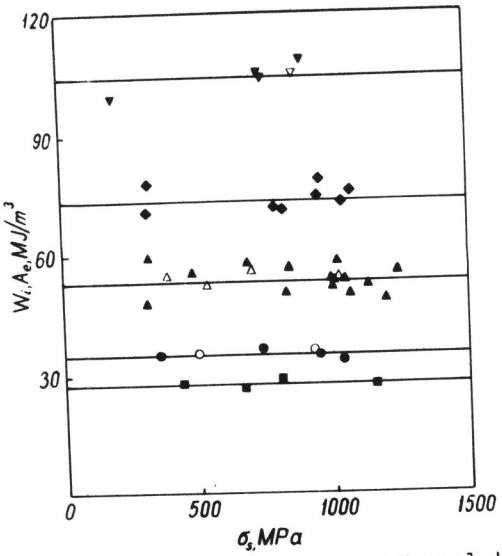

Figure 2 Threshold levels of energy W_i and the dependence of uniform deformation complete work value A_e on the lower yield point σ_s for Ti and its alloys.