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NATURE OF MASS TRANSFER IN SOLIDS UNDER CONDITIONS
OF IMPACT LOADING

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The article presents an explanation of the anomalously high mobility of atoms under the conditions of impact loading when shock waves act on a crystal.

The authors of [1-3] described a newly discovered phenomenon: when metals and alloys are exposed to short-term high-energy loads, the mobility of the atoms in the solid phase increases by many orders of magnitude.

To explain the exceedingly high migration speed of the atoms, the assumption of an interstitial mechanism of mass transfer under the given loading conditions was expressed [2]. The interstitial mechanism is perfectly compatible with the physical regularities accompanying this phenomenon, and in combination with the hypothesis of a motive force [3] it can explain the large depths of penetration of atoms upon impact loading. However, the physical meaning of the motive force remains indeterminate.

In analyzing the possible causes of the high mobility of atoms under the effect of impacts, we may eliminate the vacancy mechanism of migration of atoms from the examination, because it does not correspond to the experimental results [2]. An analogous conclusion also applies to the applicability of the model of mass transfer along dislocation canals [4] and mechanical "agitation" through the penetration of glide lamellas [5]. This, in fact, is testified to by the absence of decoration of the dislocations by traces of the disintegration of radioactive atoms on the microautoradiograms and the presence of a solid solution in the diffusion zone [3]. As regards the interstitial mechanism, the hypothesis of its applicability is compatible with the observed temperature dependence of mass transfer, and it explains the effect of the type of crystal lattice [6], the frequency of loading, and the type of solid solution [3] on the mobility of the atoms in the solid phase of metals and alloys in impact loading. However, a moving screw dislocation with jogs as a source of interstitial atoms does not ensure a sufficient number of such atoms. For instance, with a density of dislocations of 10^{10} 1/cm², the number of interstitial atoms produced by screw dislocations with jogs amounts to 0.001% of the total number of atoms in the investigated zone. Such a number of interstitial atoms is too small for obtaining the observed effects. More likely seems to be the mechanism of the formation of defects, including interstitial atoms, when a shock-wave passes through the crystal lattice of metal in explosive shock loading [7].

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We will examine in greater detail the effect of a shock-wave on mass transfer in crystalline solids exposed to impact loading, implemented, e.g., in magnetic-impact, laser, electric-pulse, and other kinds of treatment. In the experiments that were carried out, the amplitude of the shock-wave was of the order of magnitude of 10 GPa (100 kbar). To evaluate its effect on an atom situated at a lattice point (or in the interstice), we may use the equation

$$m \frac{d^2x}{dt^2} = -m\omega^2x + f(x, t). \quad (1)$$

Within the limits of atomic microvolumes

$$f(x, t) = f(t) = f_0 [\Theta(t) - \Theta(t - \tau_p)],$$

where τ_p is the time during which the disturbing force acts, equal to the time of passage of the shock front through the lattice point; $f(x, t)$ is the disturbing force induced by the stress gradient in the shock front. The numerical values of f_0 were evaluated by two methods:

$$f_0' = \frac{Vp}{l}, \quad (2)$$

$$f_0 = - \left. \frac{\partial \varphi}{\partial x} \right|_{x=x_0} \approx \frac{\varphi_2 - \varphi_1}{\delta}, \quad (3)$$

where φ_1 and φ_2 are the interaction potentials of the atoms ahead of and behind the shock front, respectively. The interaction of the atoms was described by the Born-Maier potential $\Phi = A' \exp[-\alpha(\delta - \delta_0)/\delta_0]$. With the values of the parameters $A' = 0.053$ eV; $\alpha = 13.9$; $\delta_0 = 2.866$ Å [8, 9], the potential describes well the elastic properties of copper and the energy characteristics of point defects. (In the evaluation it was assumed that $\Delta V/V_0 = 20\%$.) The solution of the equation may be written as follows:

$$x = x_{st} + \begin{cases} \frac{f_0}{m\omega^2} [\cos \omega(t - \tau_p) - \cos \omega t], & t < \tau_p, \\ \frac{f_0}{m\omega^2} [1 - \cos \omega t], & t \geq \tau_p. \end{cases} \quad (4)$$

If we use formulas (2)-(4) for the numerical evaluation of the maximum displacement of an atom from the lattice point, we obtain that $x_{\max} > \delta$, i.e., it exceeds the interatomic distance. Such an evaluation permits the assumption that the atoms of the crystal lattice abandon their lattice points in the zone through which the shock-wave passes, and the short-range and long-range orders of the crystal lattice will be disturbed. That the atoms leave the nodes of potential wells is also testified to by the fact that the perturbation energy of the atoms at the point $E^* \sim \Delta \varphi = 0.8$ eV is close to the energy of vacancy formation $E_v = 0.81$ eV [10], $E_v = 0.9$ eV [11], and $E_v = 1$ eV [12]. These evaluations are confirmed by the experimental results obtained by the authors of [13, 14]. According to these authors, local heating in the shock front amounts to 10^4 °K (for Plexiglas). For transparent ionic crystals temperatures of the same order of magnitude were obtained. Kormer [14] also finds a connection between disturbance of the crystal lattice in the shock front and increased electrical conductivity in ionic crystals when shock-waves of sufficient intensity ($p > 17$ GPa) pass through. Thus, on the basis of evaluations and of the analysis of the experimental results of [13, 14] it may be assumed that when a shock-wave of sufficient intensity ($f_0/m\omega^2 > \delta$) passes through a crystal, a zone of local disturbance of the crystalline order forms in the front of this wave, and this zone then moves at the speed of wave propagation; its size is of the order of magnitude of the width of the shock front in a solid. When $f_0/m\omega^2 > \delta$, there is a zone of high concentration of defects in the shock front because the force f_0 acting on the atom lowers the formation energy of point defects of the crystal lattice.

Since outside the shock front the processes of migration of atoms differ only slightly from steady state and equilibrium, and at low temperatures there are practically none, the responsibility for mass transfer in impact events is ascribed to processes occurring in the zone of disorder. Because of the strong blurring of the unloading wave front, the disturbance of the motion of the atoms, caused by the wave in the crystal lattice, is not great and may be neglected. We will analyze the possibility of a flux of atoms existing in the zone of the

shock-wave. For that we obtain an equation of the flux of tagged atoms in the zone of disorder (we assume that l_t is constant), analogous to the flow equation in electron transfer presented in [15]:

$$J^{(*)x} = c^*(0) \sum_{i=1}^2 l_{i0i} \left[\frac{1}{\tau'_{0i}} - \frac{1}{\tau_{i0}} \right] - \frac{\partial c^*(0)}{\partial x} \sum_{i=1}^2 l_{i0i}^2 \frac{1}{\tau'_{0i}}, \quad (5)$$

where the summing index indicates positive $i = 1$ and negative $i = 2$ direction of the jump of an atom from point 0 along the x axis.

Since the relaxation time of the distribution function to distribution of local equilibrium [16] $\tau = 10^{-13}$ sec is much shorter than the characteristic time interval of mass transfer $\tau_p \sim 10^{-11}$ sec, it may be assumed that in the zone of crystalline disorder a Maxwell-Boltzmann distribution is established. Then in the case of a shock-wave of high intensity ($f_0/m\omega^2 > \delta$) we may write for the probability of an atomic jump in the zone of crystalline disorder:

$$\frac{1}{\tau'} = c^* \frac{1}{\tau} A \exp\left(-\frac{xf_0}{kT}\right) \int_{v_m}^{\infty} \exp\left(-\frac{mv^2}{2kT}\right) dv. \quad (6)$$

Taking (6) into account, and also $l_{t0i} = -l_{t_{i0}}$ and $l_{t_{01}} = -l_{t_{02}}$, we write Eq. (5) as follows:

$$J^{(*)x} = 4Ac^*v_m \operatorname{sh}\left(\frac{f_0 l_t}{kT}\right) \int_{v_m}^{\infty} \exp\left(-\frac{mv^2}{2kT}\right) dv - 4A \frac{l_t^2}{\tau} \frac{\partial c^*}{\partial x} \operatorname{ch}\left(\frac{f_0 l_t}{kT}\right) \int_{v_m}^{\infty} \exp\left(-\frac{mv^2}{2kT}\right) dv. \quad (7)$$

If a shock-wave of low intensity ($f_0/m\omega^2 < \delta$) passes when there is a high concentration of point defects in the front of this wave, then the force f_0 will act on the defects, and this will change the activation energy of their motion [17]. Using the equation of the flux in the case of force f_0 acting in a bcc crystal [15], we write the equation of the flux of tagged atoms in the zone of high concentration of point defects, migrating by the vacancy $J_V^{(*)x}$ and the interstitial $J_I^{(*)x}$ mechanism, for a crystal with cubic lattice:

$$J_V^{(*)x} = -2\delta v \exp(-Q_V/kT) c_V c^* \operatorname{sh}\left(\frac{\delta f_0}{kT}\right) - \frac{\delta^2}{2} v \exp(-Q_V/kT) \frac{\partial c^*}{\partial x} c_V \operatorname{ch}\left(\frac{\delta f_0}{kT}\right), \quad (8)$$

$$J_I^{(*)x} = 2\delta v \exp(-Q_I/kT) c^* c_I \operatorname{sh}\left(\frac{\delta f_0}{kT}\right) - \frac{\delta^2}{2} c_I \frac{\partial c^*}{\partial x} v \operatorname{ch}\left(\frac{\delta f_0}{kT}\right) \exp(-Q_I/kT). \quad (9)$$

Since $Q_V \gg Q_I$, then $J_V^{(*)x} < J_I^{(*)x}$; consequently, the summary flux is determined by the value of the flux of interstitial atoms; this is in agreement with the hypothesis expressed in [3]. With increasing intensity of the shock-wave, the temperature in the wave front increases, and so does the ratio $J_V^{(*)x}/J_I^{(*)x} = \gamma$. When the characteristic of the shock-wave approaches values satisfying the relation $f_0/m\omega^2 \sim \delta$, the concentration of point defects attains 100%, $\gamma \rightarrow 1$. Thus, in a shock front there is an atomic flux that determines the high rate of blurring of the concentration profiles; this was also observed experimentally by the authors of [1-3]. The suggested scheme of the process of mass transfer confirms the hypothesis of the interstitial mechanism of mass transfer [2, 3] when impact loads exciting shock-waves of low intensity act, and this endows the motive force of mass transfer with real physical meaning (formulas (2), (3)). Thus, if we examine the effect of a shock-wave on a crystal, we may describe the high mobility of the atoms without using large mass-transfer coefficients.

Taking (7) and (9) into account, we may write the continuity equation of the flux for the zone of the shock-wave:

$$\frac{\partial c^*}{\partial t} = -\frac{\partial J^{(*)x}}{\partial x}, \quad (10)$$

which is the equation of mass transfer in the front of this wave. For describing the process of macromass transfer in a crystal, it is necessary to solve the problem of mass transfer for a bounded body with specified initial distribution, taking into account the motion of the zone and the change of the initial boundary conditions in its motion. The dimension of the body will be the dimension of the zone in the shock front.

NOTATION

t, time; T, temperature; m, atomic mass; x, linear coordinate; k, Boltzmann constant; φ , potential; $f(x, t)$, disturbing force; f_0 , disturbing force in the shock front; w, oscillation frequency of an atom in the lattice point; $\Theta(t)$, Heaviside function; V, volume of an elementary cell of the crystal lattice; p, pressure in the shock wave; l , width of the shock front; δ , lattice parameter; τ_p , time of the disturbing force acting; τ , relaxation time of the distribution function to local equilibrium distribution; E^* , energy of atom disturbance in a lattice point; E_v , energy of vacancy formation; τ' , time of atom jump in the direction of the OX axis; v_m , most probable speed of the atom in the zone of the lattice disorder; A, constant normalizing the distribution function; $J^{(*)x}$, flux of tagged atoms migrating in the shock front; c^* , concentration of tagged atoms; c_v , concentration of vacancies; c_i , concentration of interstitial atoms; l_t , free path in the zone of lattice disorder; Q_v , activation energy of vacancy motion; Q_i , activation energy of the motion of an interstitial atom; ν , frequency of Debye order; γ , parameter of the ratio of fluxes of tagged atoms in the shock front effected by the vacancy and interstitial mechanisms; x_0 , coordinate of the shock front.

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