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Transfer of Interstitial Atoms under Elastic Shock Deformation of the Metal Surface

A. I. Karasevskii and A. Yu. Naumuk

G. V. Kurdyumov Institute for Metal Physics, N.A.S. of Ukraine,
36 Academician Vernadsky Blvd.,
UA-03142 Kyiv, Ukraine

The process of anomalous transfer of interstitial atoms during impact deformation of the crystal surface is described theoretically. As shown that surface impact leads to the formation in the crystal of a wave of inhomogeneous atomic displacements, which propagates from the surface into the crystal depth. The formation of a deformation wave leads to a change in the interatomic distance at the wave front and a change in the potential energy for interstitial atoms. As well, interstitial atoms at the front of the deformation wave receive an additional impulse, which leads to an increase in their kinetic energy and contributes to the activationless (emission) transfer of atoms deep into the crystal.

Key words: emission transfer of interstitial atoms, impact deformation, deformation wave, potential energy of interstitial atoms.

Теоретично описано процес аномального переносу міжвузлових атомів за ударної деформації поверхні кристала. Показано, що поверхневий удар призводить до формування в середовищі хвилі неоднорідних атомних зсувів, яка поширюється від поверхні в глибину кристала. Утворення деформаційної хвилі призводить до зміни міжатомної відстані на фронті хвилі, внаслідок чого змінюється потенціяльна енергія міжвузлових атомів. Крім того, міжвузлові атоми на фронті деформаційної хвилі отримують додатковий імпульс, що призводить до зростання їхньої кінетичної енергії і сприяє емісійному (безактиваційному) просуванню атомів вглиб кристала.

Corresponding author: Anatoliy Illich Karasevskii
E-mail: akaras@imp.kiev.ua

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Ключові слова: аномальне перенесення міжвузлових атомів, ударна деформація, деформаційна хвиля, потенціяльна енергія міжвузлових атомів.

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1. INTRODUCTION

The impact of radiation on the surface of a metal or semiconductor at sufficiently high radiation energy can lead to the escape of electrons or ions from the medium. This occurs when the radiation energy transferred to the charge exceeds the work function of the charges from the medium. A number of works (see, for example, [1–3]) revealed a significant increase in the rate of mass transfer of interstitial atoms in a metal under shock loading of its surface. In this case, the impact can be of a different nature—mechanical shocks, laser pulses, spark discharges and the like. For the theoretical description of anomalous mass transfer, a number of models have been proposed, the most developed of which are the dislocations models [4–6]. Within the framework of this model, it is assumed that an interstitial atom is captured by a dislocation and transported by it at macroscopic distances deep into the crystal.

In this work, it is shown that surface impact leads to the formation in the crystal of a wave of inhomogeneous atomic displacements, propagating from the surface into the depth of the crystal. That leads to a change in the interatomic distance at the front of the deformation wave, and changes the relief of the potential energy for interstitial atoms. In addition, interstitial atoms at the front of the deformation wave receive an additional impulse, which increases their kinetic energy and helps the atoms to overcome of interstitial potential barriers. When the increasing in the kinetic energy of interstitial atoms exceeds the value of the potential barrier, the mechanism of atomic transfer changes from of the activation to emission one.

2. SHOCK WAVES OF LONGITUDINAL DISPLACEMENTS

An impact on a flat crystal surface located perpendicular to the axis x initiates the appearance of quasi-one-dimensional longitudinal waves of displacements of crystal atoms $u(x, t)$, the evolution of which is described by the hyperbolic equation [7]:

$$u_{tt} = a^2 u_{xx}. \tag{1}$$

The function $u(x, t)$ represents at the moment t the displacement of a

point having an abscissa x in the equilibrium position, u_{tt} and u_{xx} the second derivatives of the displacements with respect to time and coordinate, $a = (k/\rho)^{1/2}$ is the speed of sound in the rod, k is Young's modulus, and ρ is the density of the medium. The relative elongation of the sample at a point x is equal to $u_x(x, t)$.

We will consider a metal rod with a length l, rigidly fixed at the origin of coordinates ($u(0, t) = 0$), which until time $t = 0$ is in equilibrium ($u(x, t) = 0$, $t \le 0$). The free end of the rod ($u_x(l, t) = 0$) at the initial moment of time receives a longitudinal shock impulse I:

$$u_t(x, 0) = -\frac{I}{\rho}\delta(x - x_0),\ 0 < x_0 < l,\ x_0 \to l. \tag{2}$$

To solve equation (1), we will use the method of separation of variables [7] that put

$$u(x, t) = X(x)\,T(t). \tag{3}$$

Substituting (3) into (1), taking into account (2), and, the above mentioned initial and boundary conditions, we obtain:

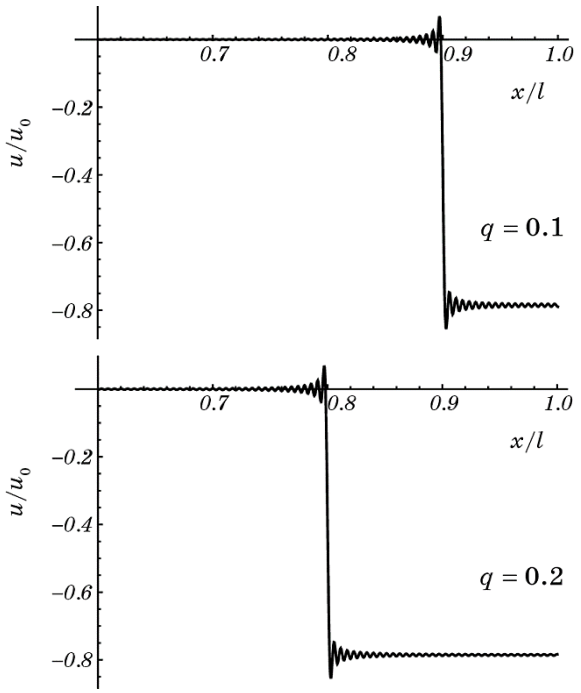
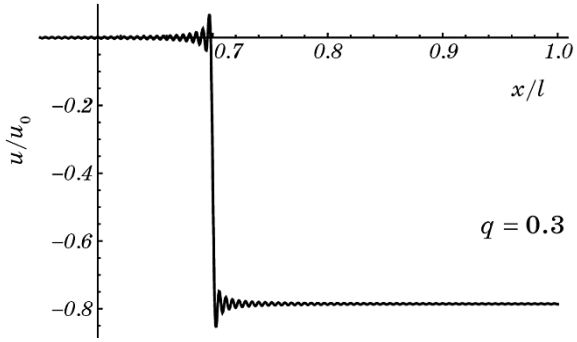


Fig. 1. Dependence of the reduced value of the displacement $u(x, t)/u_0$ on the dimensionless coordinate $\eta = x/l$ at different points in time $q = (a/l)t$.



Continuation of Fig. 1.

$$u(x,t) = -\frac{2I}{\pi a \rho} F(q,\eta), \tag{4}$$

where

$$F(q,\eta) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)} \left(\cos\left[\frac{(2n+1)\pi}{2} (\eta - q) \right] - \cos\left[\frac{(2n+1)\pi}{2} (\eta + q) \right] \right). \tag{5}$$

Figure 1 shows the dependence of the reduced value of the displacement $u(x, t)/u_0$ on the dimensionless variables of time $q = (a/l)t$ and coordinates $\eta = x/l$, where $u_0 = 2I/(\pi a \rho)$. From formulas (4), (5) and Fig. 1, it follows that after the impact, a deformation wave with a sharp front and constant amplitude is formed in the crystal, which propagates into the depth of the crystal without distortion. The speed of movement of the deformation wave front $u(x, t)$ is equal to a. The position of the shock front is determined by the relation $\eta_{Fr} = 1 - q$.

3. CHANGES IN THE MICROSTRUCTURE OF A CRYSTAL IN THE FIELD OF A SHOCK WAVE

Consider a metal rod with a crystal structure of a simple cubic lattice ($a_0 = b_0 = c_0$). Let the lattice constant in the non-deformed state be $2a_0$ (see Fig. 2).

After hitting on the end surface of the bar ($x = l$), the physical point of the bar, which at the initial moment occupies the position x, at any subsequent moment t will be at the point with the coordinate $X = x + u(x, t)$ (see, *e.g.*, [7]). As a consequence, the lattice constant in the sample will be equal to [7]

$$2a = 2a_0 + u(x + 2a_0, t) - u(x, t).$$

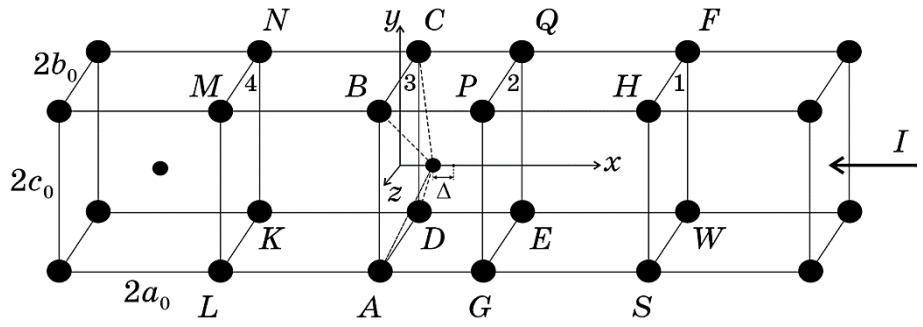


Fig. 2. Displacement of atoms of a cubic lattice during the passage of a deformation wave.

In the region of uniform deformation of the sample ($x > G$), $u(x + 2a_0, t) \approx u(x, t)$, the lattice constant does not change $a = a_0$ (Fig. 2).

To the left of the front boundary ($x \le G$) $u(x, t) = 0$, and the grating constant at the wave front (*AG* layer in Fig. 2) is

$$a_{AG} = 2a_0 + u(x_G, t). \tag{6}$$

Since, $u(x_G, t) < 0$, the interatomic distance in the layer of atoms, which is adjacent to the front of the deformation wave, decreases, that is the medium at the wave front is compressed. Local dynamic compression of the medium (atomic layer *AG* in Fig. 2) will lead to a change in the potential relief and kinetic energy of the interstitial atom. This can be shown by direct calculation.

Let's choose the origin of coordinates in the centre of the plane *ABCD*, in which we place the coordinate axes *YZ*. The initial position of the interstitial atom will be determined by the coordinates $\{a_0 + u - \Delta, 0, 0\}$, where

$$X_{\text{at}} = a_0 + u - \Delta \tag{7}$$

is the position of the interstitial atom on the *X*-axis, Δ is parameter that determines the current position of the atom. So, for example, in equilibrium when the atom is in the centre of the cell ($X_{\text{at, 0}} = a_0$), $\Delta = 0$.

The interaction of an interstitial atom with atoms of the matrix will be approximated by the Lennard–Jones potential:

$$U(R_{s,j}) = 4\varepsilon \left[\left(\frac{\sigma}{R_{s,j}} \right)^{12} - \left(\frac{\sigma}{R_{s,j}} \right)^{6} \right], \tag{8}$$

where $R_{s,j} = |\mathbf{R}_s - \mathbf{R}_j|$ is the distance between the interstitial atom *s* and the *j*-th atom of the crystal.

The potential energy of an interstitial atom is determined by the energy of its interaction with the crystal atoms (8). And transfer of an atom under the influence of a deformation wave from the near-boundary crystal cell AG to the neighbouring undeformed cell LA will be accompanied by a change in its potential energy.

We restrict ourselves to taking into account the interaction of the interstitial atom with the atoms of the matrix, which are located in 1, 2, 3, and 4 planes of the crystal lattice (Fig. 2). The distances between an interstitial atom and atoms located in the 1, 2, 3, and 4 planes of the crystal are

$$R(1) = a_0\sqrt{\left(3+\frac{\Delta}{a_0}\right)^2+2},\ R(2) = a_0\sqrt{\left(1+\frac{\Delta}{a_0}\right)^2+2},$$
$$R(3) = a_0\sqrt{\left(1+\frac{u-\Delta}{a_0}\right)^2+2},\ R(4) = a_0\sqrt{\left(3+\frac{u-\Delta}{a_0}\right)^2+2}, \tag{9}$$

$$\frac{U(\chi,\gamma)}{16\,\varepsilon} = s^{12}\left([(3+\chi)^2+2]^{-6}+[(1+\chi)^2+2]^{-6}+[(1+\gamma-\chi)^2+2]^{-6}+\right.$$
$$\left.+[(3+\gamma-\chi)^2+2]^{-6}\right)-s^6\left([(3+\chi)^2+2]^{-3}+[(1+\chi)^2+2]^{-3}+\right. \tag{10}$$
$$\left.+[(1+\gamma-\chi)^2+2]^{-3}+[(3+\gamma-\chi)^2+2]^{-3}\right),$$

where $\chi = \Delta/a_0$, $\gamma = u/a_0$, $s = \sigma/a_0$.

In the equilibrium state before striking ($I = 0$, $u = 0$), the distribution of the potential energy of an interstitial atom in neighbouring cells LA and AG is symmetric with respect to the plane $ABCD$ (Fig. 3).

After impact on the sample surface, the potential barrier for the

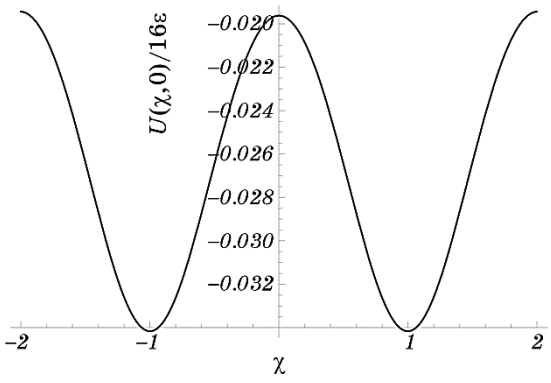


Fig. 3. Equilibrium distribution of the potential energy of an interstitial atom $I = 0$, $u = 0$, $s = 0.8$.

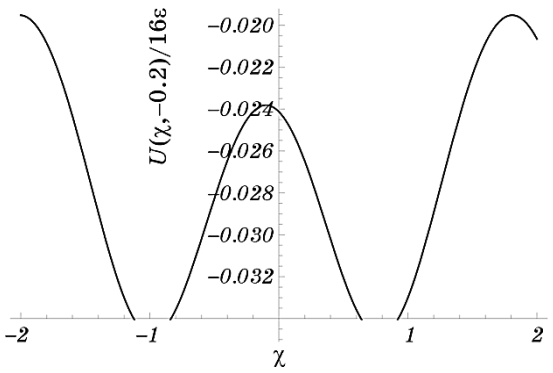


Fig. 4. At a small value of the deformation pulse I ($s = 0.8$, $u = -0.2$), the potential barrier to the transfer of interstitial atoms at the wave front decreases.

transition of atoms in the direction of impact, decreases (Fig. 4).

At a larger longitudinal momentum, the barrier separating the localized states of an interstitial atom practically disappears (Fig. 5).

4. EMISSION FLUX OF INTERSTITIAL ATOMS IN THE FIELD OF A SHOCK

Under impact deformation of the crystal surface, part of the longitudinal momentum I is transferred to the interstitial atom. This leads to an increase in its kinetic energy and makes it easier for the atom to overcome the potential barrier separating neighbouring localized states.

The speed that an interstitial atom acquires due to its interaction

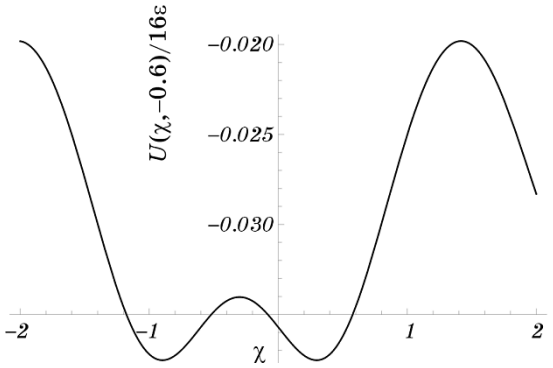


Fig. 5. With a significant value of the deformation impulse I, the potential barrier practically disappears $s = 0.8$, $u = -0.6$.

with the front of the deformation wave is

$$V_{\text{at}} = \frac{\partial X_{\text{at}}}{\partial t} = \frac{\partial u(x,t)}{\partial t}. \tag{11}$$

Considering that $q = (a/l)t$,

$$\frac{\partial u(x,t)}{\partial t} = \frac{2I}{\pi\rho l}\frac{\partial F(q,\eta)}{\partial q}, \tag{12}$$

where $F(q, \eta)$ is determined by expression (5). To find the derivative $\partial F(q, \eta)/\partial q$ at the front of the deformation wave, $\eta_{\text{Fr}} = 1 - q_0$, $q_0 = (a/l)t_0$, the easiest way is to use numerical methods, assuming

$$\left.\frac{\partial F(q,\eta)}{\partial q}\right|_{q\to q_0} = \left.\frac{F(q_0 + \Delta q) - F(q_0)}{\Delta q}\right|_{\Delta q\to 0}. \tag{13}$$

As follows from (12) and Figure 6, at the front of the deformation wave, the velocity of the longitudinal (from right to left) motion of the interstitial atom increases, which leads to an increase in its kinetic energy, the value which can exceed the value of the activation barrier separating the minima of the potential energy of the interstitial atom in neighbouring cells for example *LA* and *AG*. The additional kinetic energy that receives, while the interstitial atom of mass m is equal to

$$E_K = \frac{2mI^2}{\pi^2\rho^2 l^2}\left(\frac{\partial F}{\partial q}\right)^2. \tag{14}$$

Taking into account that $I = M_0 V_0$, $\rho l = M$, expression (14) can be rewritten as

$$E_K = \frac{2}{\pi^2} m V_0^2 \left(\frac{M_0}{M}\right)^2 \left(\frac{\partial F}{\partial q}\right)^2\Bigg|_{q\to q_0}. \tag{15}$$

As an example, we put

$$m = 9.3\,10^{-23}\,\text{g},\ V_0 = 10^3\,\text{cm/s},\ M_0/M = 5,\ (\partial F/\partial q)|_{q\to q_0} = -80,$$

then $E_K = 1.9$ eV, that is, the value of E_K is comparable (or more) to the value of interstitial potential barriers. If the value E_K exceeds the value of the activation barrier that an interstitial atom needs to overcome in order to enter the neighbouring cell, then the process of atom moving occurs without activation and emission of interstitial atoms into the bulk of the crystal occurs.

It will be emphasized that an increase in the longitudinal momentum

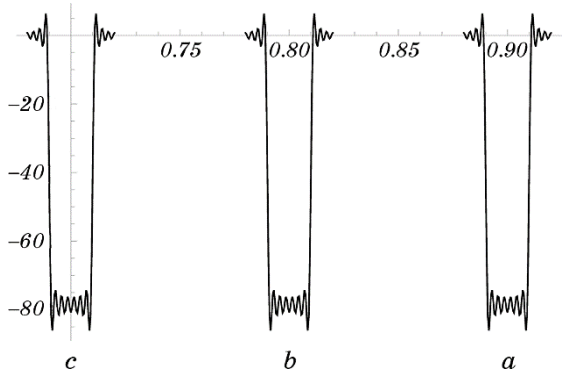


Fig. 6. The value of the derivative (13) at different positions of the deformation wave front: $\eta_{Fr} = 0.1$ (*a*), $\eta_{Fr} = 0.2$ (*b*), $\eta_{Fr} = 0.3$ (*c*).

leads not only to an increase in the kinetic energy of an interstitial atom, but also significantly lowers the activation barrier for atomic transfer.

5. RESULTS AND DISCUSSION

As already noted, the radiation effect on the surface of a metal or semiconductor can lead to the escape of electrons or ions from the medium. This occurs when the radiation energy that is transferred to the charge exceeds the work function of the charges from the medium. A classic example of emission is the emission of electrons from metals and semiconductors, when, under the influence of an electromagnetic wave, part of the electrons passes into the conduction band (internal photoelectric effect) or leave the medium (external photoelectric effect).

A similar situation will be observed in the case of the appearance of a deformation wave in a crystal containing interstitial impurity atoms. Upon impact on the surface of the crystal, the atoms of the crystal are elastically displaced layer by layer, without dissipative transfer of the energy of elastic deformation into the interior of the crystal. The presence of an interstitial impurity atom in the crystal lattice breaks the translational symmetry of the lattice and leads to scattering (absorption) of the elastic wave energy. When the value of the absorbed energy exceeds the energy of localization of an interstitial atom in the crystal, the emission of the interstitial atom into the bulk of the crystal occurs.

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