

## EVOLUTION OF CRYSTAL MORPHOLOGY UNDER FLOW OF LOW-ENERGY PARTICLES: VACANCY MECHANISM

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**Abstract.** Initial stages of a crystal surface morphology evolution under local impact of low-energy (of the order of eV and even less) particle beam were studied and a simulation of this process was performed using molecular dynamics. It is shown that change in the crystal morphology can be caused by a vacancy flow towards the spot of the beam incidence along crystallographic directions corresponding to phonon propagation. The mathematical model of this process is proposed and surface profile change rate is estimated. A mechanism of surface roughness development on initially flat surface under impact of uniform particle flux over the whole area is discussed, and morphological stability criterion is found. It is shown that in certain cases one can smooth the surface of the crystal overcoming other mechanisms of spontaneous roughness development.

### 1. Introduction

Nowadays a lot of attention is paid to study of destruction and change in morphology of crystals [1, 2] under impact of different external factors: mechanical load [3, 4], heating, and laser irradiation [5]. Also mechanisms of destruction of crystals treated by ionic beams and beams of other particles are of interest. Generally, in these studies the change in morphology is caused by one of the following processes: thermal destruction due to local heating of both the sample and absorbing inclusions in its volume; avalanche ionization [6]; various thermochemical processes; mechanochemical phenomena; formation and accumulation of different lattice defects and their subsequent migration. Detailed discussion of these and other mechanisms is presented in reviews [7, 8, 9]. Usually in studies on a particle beam impact high-energy particles in the range of 0.1 - 100 keV [7] are considered, which is much higher than the binding energy of atoms in a crystal (a few eV). Selection of this range is determined by the fact that collisions of such particles with the crystal surface heat it effectively, knock out atoms from the surface [10], and lead to formation of various defects in the volume. The method of molecular dynamics (MD) is frequently used for consideration of these processes [11]. MD within atomistic approach allows one to describe the interaction of the incident particles with the surface and calculate local values of various parameters: temperature and average displacement of atoms from equilibrium position. One of the advantages of this method is that it allows observing such phenomena as generation and movement of defects, for example, formation of craters on the surface and pores in the crystal volume, movement of interstitial atoms, vacancies and many

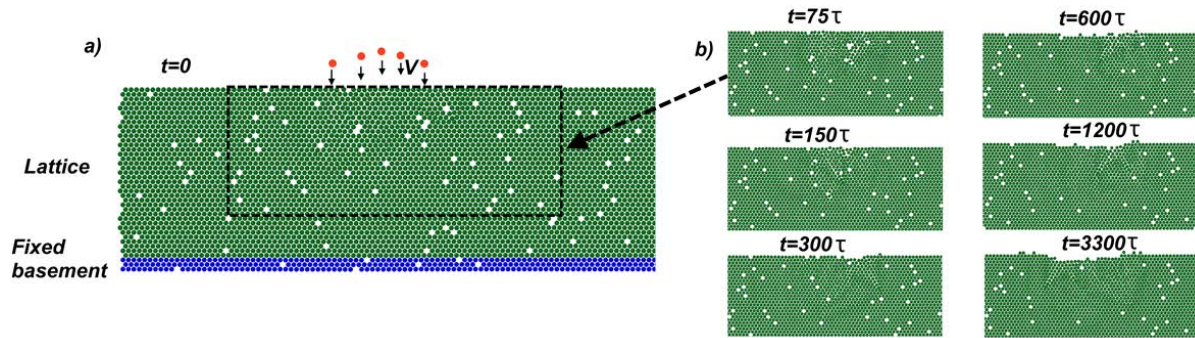
others [12]. In this paper we studied the interaction of the particle beam with the crystal surface using MD and detected a mechanism differing from the abovementioned mechanisms. It leads to a change in surface morphology of the crystal under the flow of particles even of low energy, which is comparable to the activation energy of vacancy migration ( $\sim 0.1-2$  eV). This mechanism is not related directly to heating, knocking out of atoms from the surface and creation of defects in the crystal volume, but is associated with a flow of vacancies from the bulk of the crystal towards the spot of beam incidence. The mechanism can lead to a gradual change of the surface relief even if cooling of the sample is efficient and beams' intensity is low. The first part of the paper is devoted to study of the local morphology change under a point impact of the beam. The main objective of the second part is the consideration of influence of discovered mechanism on the development of surface roughness under uniform irradiation of the entire sample by the beam of particles [9]. We will show that the mechanism can in some cases lead to growth of an arbitrarily small perturbation on the crystal surface accounting for development of roughness, while in other cases, conversely, can result in smoothing the surface. This phenomenon can be used in processing of thin films and crystals in order to obtain smooth surfaces.

## 2. The mechanism of change in the crystal morphology: simulation by MD

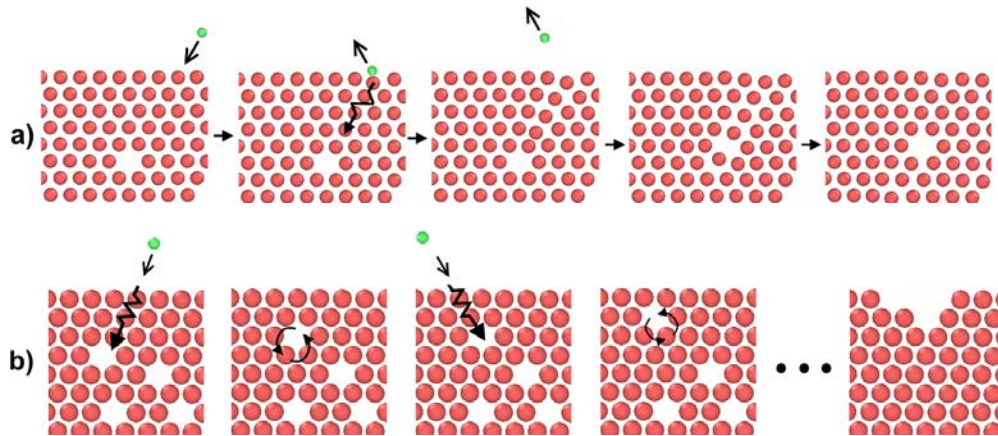
Simulation was performed by the method of molecular dynamics. For a qualitative understanding of processes occurring in the crystal, we considered beams of neutral atoms over a wide energy range falling on the surface. With a decrease in energy and intensity of the falling particles, traditional mechanisms of destruction of the crystal such as local heating and knocking out of the surface atoms [9], penetration of particles into the volume of the crystal, formation of defects and ballistic diffusion gradually ceased to affect the surface morphology. At particle energies comparable to the binding energy of atoms in the crystal or smaller, a different mechanism has been revealed in which the surface morphology changes gradually due to a flux of vacancies from the bulk of the crystal towards its surface. The simulation was performed in LAMMPS software package [13] and visualization in OVITO package [14]. We considered 2-dimensional rectangular crystal on a fixed basement. The crystal was represented by hexagonal lattice (see Fig. 1a), containing 4400 atoms, whose interaction is described by the Lennard-Jones (LJ) potential  $E = 4\epsilon[(\sigma/r)^{12} - (\sigma/r)^6]$ . The calculations were performed in the reduced dimensionless system of LJ units, which are often used in MD [15], with parameters  $\epsilon = 1$ ,  $\sigma = 1$ , and the cutoff radius of  $2.5 \sigma$ . The mass of the atoms in the lattice was  $m_a = 1$ . For the incident beam we used light particles ( $m_p = 0.05$ ), which were generated in a specific area (see. Fig. 1a) above the surface with a time period of  $2.5 \tau$ , and with a normal velocity of incidence  $v = -5 \sigma / \tau$ . Thus, the energy of the incident particles was equal to  $0.625 \epsilon$ , which is significantly less than the binding energy of an atom on the surface with its neighboring atoms. After collision and transmission of the momentum to the crystal surface, these particles were removed from the system. Time step was  $dt = 0.005 \tau$ . The initial temperature of the system was chosen rather low and amounted  $T = 0.1 \epsilon$ . Every 100 steps we scaled speed of all atoms in a way that the temperature remained the same, i.e. system was thermostated. Figure 1b shows the evolution of the system at different times.

One can note that over time vacancies drift from the volume towards the crystal surface forming a crater. A more detailed mechanism of vacancy drift can be described as follows. After a collision of the low-energy particle with the surface it is reflected giving the part of the momentum to the lattice. This may result in arising phonons which will probably propagate into the crystal (see Fig. 2). Phonon energies in real crystals are within the range of  $0.01-0.1$  eV [16, 17], which is comparable with the vacancy migration energy for certain substances ( $0.1-2$  eV

[18, 19, 20]). Thus, during the scattering of a phonon on the vacancy it is possible that the last atom involved in a collective oscillation of the atomic chain will hop into the vacancy site. Therefore, vacancy will become closer to the surface by one interatomic distance (see Fig. 2a). This polyatomic process is similar to the Newton pendulum [21], where impact on the first atom in a polyatomic chain leads to transfer of momentum to the last atom, forcing it to move into subsequent vacancy site. In case when the next phonon is scattered on the same vacancy, it can again make a hop. Thus, under the influence of the phonon field vacancies will drift towards the source of phonons, i.e. to the surface. The preferential direction of their movement will correspond to the crystallographic directions of phonon propagation. Via this mechanism, vacancies will gradually accumulate in the surface region where the particle beam falls forming pores or holes which will continue to increase in size due to further inflow of vacancies (see Fig. 2b).



**Fig. 1.** Two-dimensional hexagonal crystal lattice containing vacancies and a flux of low-energy particles onto it (a). Temporal evolution of the vacancy distribution and surface morphology near the spot of beam incidence (b).

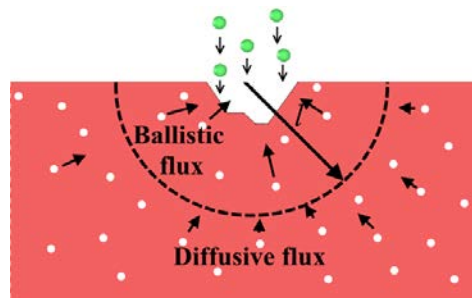


**Fig. 2.** Mechanism of vacancy hopping towards the place of incidence of the particle (a), and schematic view of the gradual change in crystal surface morphology under impact of low-energy particles (b). As a result of generation and propagation of phonons vacancies drift to the surface.

### 3. Change in the crystal surface morphology under local impact of the beam: mathematical model

A simplified mathematical model was developed to describe the revealed mechanism, which is presented below. It should be noted that within the atomistic approach we do not take into account electron-phonon interactions, formation of polarons and other phenomena associated

with the electronic subsystem, thus considering only the mechanical interaction of atoms and particles. Let us assume for simplicity that intensity of the flux of particles is sufficiently small, the crystal has high heat conductivity and is well thermostated because increase in local temperature may affect the thermodynamics of the crystal. We suppose that phonons have a mean free path  $l$ , which is determined by scattering on other phonons and lattice defects [22] other than vacancies. We also assume that after such scattering the phonon is no longer involved in the considered process. Let us suppose that the probability of phonon propagation in different directions is the same (though real crystal are anisotropic). If we suppose that  $l \gg R$ , where  $R$  is the lateral size of the beam of particles, then the proposed mechanism can carry away vacancies to the point of incidence only from the crystal region having a shape of hemisphere of radius  $l$  (see Fig. 3). Note that at low temperatures ( $\sim 100$ - $200$  K) in certain substances  $l$  is of the order of 1-100 microns [22] while the lateral size of the focused beam of particles in modern devices can be tens of nanometers, which makes this assumption correct. The destruction process consists of two stages (see Fig. 3). The first one is the ballistic destruction when vacancies drift to the surface due to direct interaction with phonons in the region of radius  $l$  (ballistic region). When vacancy concentration decreases in this area, the second stage begins, in which vacancy flow is caused mainly by diffusion from the bulk of the crystal to the boundaries of the ballistic region and subsequent capturing the vacancies by phonons. In Figure 1b one can see the beginning of the surface restructuring process. Also because temperature of the system is quite small and thus the diffusion coefficients of vacancies are low, the transition from ballistic mode to the diffusion mode can be traced over the time and after a while the process practically stops. The differences between the distribution of vacancies at the times  $1200 \tau$  and  $3300 \tau$  are negligible.



**Fig. 3.** Schematic view of the region in which phonons carry away vacancies towards surface (ballistic mode takes place), and the region where inflow of vacancies is determined by diffusion.

We make the assumption that particles falling on the surface are identical and lead to generation of  $Q$  lattice vibrations per second near the surface. Provided that the process takes place at temperatures below the Debye for the crystal substance, the generation of new phonons is possible. Also for simplicity we introduce variable  $p$ , which is the probability that the interaction of phonon and vacancy will lead to vacancy hopping. We assume that this integral variable takes into account such phenomena as the distribution function of energy of the phonons, arising near the surface at a given temperature, as well as the probability of vacancy hopping after its interaction with the phonon of given energy. Note that phonon scattering by point defects in particular vacancies and their clusters were studied in a considerable number of works [24, 25, 26]. We suppose that at the beginning of the process the crystal is in thermodynamic equilibrium, vacancies are distributed uniformly over the volume and their concentration is  $n_0$ . Because  $l \gg R$ , we assume that the source of the phonons is pointlike and is located at the center of the reference system ( $r = 0$ ).

**Ballistic mode.** When the beam of particles hits the surface, generation of phonons begins and they scatter on vacancies within the region of radius  $l$ , which causes drift of vacancies

towards the point of the beam incidence. Let us consider a vacancy at a distance  $r$  from that point. To reach the surface, it has to perform  $\sim r/a=k$  hopping acts, where  $a$  is a lattice parameter (length of the hop), and  $k$  is an integer. In our isotropic model the probability of phonon propagation in direction of the considered vacancy is proportional to the ratio of the projection area of the vacancy  $\pi a^2$  and a hemisphere of radius  $r$   $S=2\pi(ka)^2$ . Thus, the average hopping time of the vacancy towards the phonon source point from distance  $r = ka$  to the distance  $r = (k-1)a$  can be expressed by the following formula:

$$\frac{1}{\tau_k} = \frac{1}{2k^2} Qp.$$

Consequently, the further the vacancy is, the more time it takes to perform the hopping act. Knowing this value, we calculate the average time  $\tau_{ka}$  for vacancy to reach the surface from the depth  $r=ka$ :

$$\tau_{ka} = \sum_{k=1}^k \tau_k = \frac{2}{Qp} \sum_{k=1}^k k'^2 = \frac{1}{3Qp} k(k+1)(2k+1).$$

In the approximation that on average the distance from the spot of the beam incidence is much larger than the interatomic distance (i.e.  $k \gg 1$ ), the size of the region from which vacancies were delivered to the surface by the time  $t$ , is given by:

$$r(t) = ka \approx a \sqrt[3]{\frac{3}{2} Qpt}, \quad (1)$$

and the total number of vacancies  $F(t)$ , which reached a formed crater on the surface by this time can be estimated from the formula:

$$F(t) = \frac{2}{3} \pi r(t)^3 n_0 = \pi n_0 a^3 Qpt,$$

The flow  $J_b$  of the vacancies which joins the crater per unit time is determined by expression (2):

$$J_b = \frac{\partial F}{\partial t} = \pi n_0 a^3 Qp. \quad (2)$$

Thus, the volume of the crater increases linearly with time and its average radius  $r_y$  is proportional to the cube root of time:

$$r_y(t) = \sqrt[3]{\frac{3}{2\pi} F\Omega} = a^2 \sqrt[3]{2Qptn_0\pi},$$

where  $\Omega$  is the vacancy volume.

**Diffusion mode.** Let us consider the next stage, when radius of the region depleted by vacancies reached a mean free path  $l$  of the phonons. Quantity of vacancies  $J_D$  entrained by phonons from the boundaries of this region per unit time depends on the total number of vacancies on the boundary, which can be expressed as  $2\pi l^2 a n_l$  (where  $n_l$  is the local concentration of vacancies at distance  $l$ ).  $J_D$  is also inversely proportional to the average time  $\tau_l$  of vacancy hopping towards the phonon source and can be written as:

$$J_D|_{r=l} = \frac{2\pi l^2 a n_l}{\tau_l}. \quad (3)$$

In steady-state diffusion inflow of vacancies towards the boundaries of the region from the crystal bulk also equals to  $J_D$  and, therefore, the following equation is correct:

$$2\pi l^2 D_v \frac{\partial n}{\partial r} \Big|_{r=l} = \frac{2\pi l^2 a n_l}{\tau_l}. \quad (4)$$

Thus, it is possible to write a diffusion equation describing the concentration of vacancies  $n$  at distances  $r > l$ :

$$\frac{\partial n}{\partial t} = D_v \left( \frac{\partial^2 n}{\partial r^2} + \frac{2}{r} \frac{\partial n}{\partial r} \right), \quad (5)$$



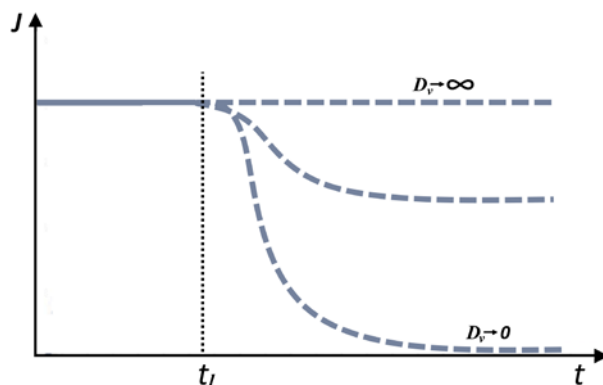
where  $D_v$  is the diffusion coefficient of vacancies in the crystal. In steady-state  $\frac{\partial n}{\partial t} = 0$  and the left-hand side of the equation (5) vanishes. Solving the equation (5) with the boundary condition for the flow and concentration of vacancies in the form of (4) and the condition at infinity ( $n = n_0$ ) one can find the distribution function of vacancies in the crystal:

$$n(r) = n_0 - \frac{n_0 l^2 a}{r(D_v \tau_l + la)}, \quad r > l \quad (6)$$

from which it is easy to deduce the desired concentration  $n_l$ . Next, using the expression (3), we can find the number of vacancies entrained from this region towards the surface per unit time:

$$J_D|_{r=l} = \pi n_0 a^3 Q p \left[ 1 - \frac{Q p a^3}{(2D_v l + Q p a^3)} \right]. \quad (7)$$

From the equation (7) it follows that if the diffusion coefficient is small, the concentration of vacancies at the boundary becomes extremely low and the growth of the crater practically stops, as can be seen in Figure 1b. If the diffusion takes place actively, the flow of vacancies in steady-state becomes approximately  $(1 - Q p a^3 / 2D_v l)$  times smaller than in the initial ballistic mode. The time dependence of the flow  $J$  of the vacancies towards the crater (corresponding to the rate of change of the surface profile) is shown in Fig. 4. The transition from the ballistic to the diffusion mode takes place at time  $\tau_l$ , which is determined by the phonon mean free path  $l$  by the expression (1) (if one substitute  $r = l$ ). Thus, by measuring this time we can estimate  $l$ . If we know the ratio of destruction rates in the ballistic and in the diffusion modes, and certain parameters of the crystal (such as lattice parameter  $a$ , the diffusion coefficient  $D_v$ ,  $l$  etc.), we can estimate the unknown values of  $Q$  and  $p$ .



**Fig. 4.** Time evolution of vacancy flow  $J$  towards the crater via considered mechanism for different diffusion coefficients of vacancies  $D_v$ .  $t_l$  is the average drift time of vacancy to the surface from the distance equal to the phonon mean free path  $l$ .

It should be noted that by applying to the crystal tensile or compressive mechanical stresses, one can significantly affect the equilibrium concentration of vacancies  $n_0$  [3] increasing or decreasing it, respectively. From the formulas (2) and (7) one can conclude that change in morphology of the crystal will proceed more efficiently on the samples subjected to tensile stresses because of higher vacancy concentrations. However, when mechanical stresses are applied to the system, the spontaneous development of surface roughness can occur, which is discussed in the next section.

#### 4. Development of surface roughness under uniform impact of particle beam on the elastically strained crystal

In the previous section, we considered local morphology change under the influence of the particle beam at a certain point at the surface. Let us now consider how the surface profile

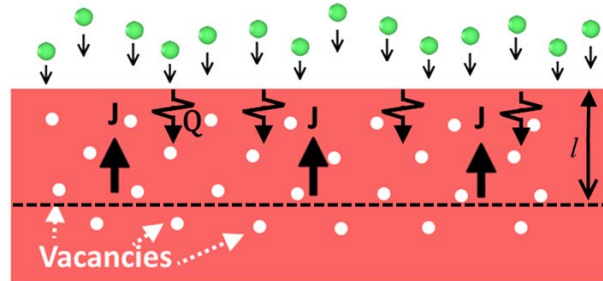
changes when the particle beam uniformly influences the entire sample, and how spontaneous development of roughness can occur. Morphological stability theory developed in the classical work of Mullins and Sekerka [27], is often used to study such processes and to determine the stability criterion of the surface with respect to random fluctuations of the form. Within the framework of this theory a small perturbation of the form is imposed on the investigated surface and its temporal evolution under the influence of various factors is being studied. Comparing different mechanisms of shape transformation, it is possible to find a criterion of spontaneous overgrowth of arbitrary small perturbation of surface. To date, the stability of the spherical [27], cylindrical [28], flat and other surfaces has been studied and the effect of different phenomena on the stability has been investigated. The considered phenomena included anisotropy of surface tension [29], diffusion of adatoms on the surface and in the bulk crystal, mechanical stress and diffusion of vacancies [30], presence of chemical reactions in multi-component systems [31], and desorption of adatoms [32].

To find spontaneous roughness development criteria, let us consider a flat elastically-strained crystal surface. The elastic stresses  $\sigma$  might be caused by a number of factors, for example the presence of large subsurface lattice defects or, in case of thin films which are often used in production of semiconductor devices, the presence of foreign substrate with a different lattice parameter [33].

The flux of vacancies  $J$  towards the surface after beginning of the beam exposure (see Fig. 5) can be calculated as follows. The number of vacancy hopping acts per unit time within the atomic layer of thickness  $a$  on arbitrary depth  $h < l$  through the area  $S$  is proportional to  $Q$  [ $m^{-2}$ ], the integral probability  $p$ , introduced in the previous section, as well as to probability of propagation of phonon in direction of one of the  $N = n_0 Sa$  vacancies located in this layer within the area  $S$ . The latter probability can be estimated as the ratio of the total area of the projection of  $N$  vacancies ( $Na^2$ ), to the full area  $S$  because we assume that vacancies in different atomic layers do not “shadow” one another

$$J = Qp \frac{Na^2}{S} = Qpn_0a^3. \quad (8)$$

Note that since all the atomic layers at depths of less than  $l$  are alike in terms of interaction with phonons and have on average the same number of vacancies. As soon as any vacancy in some layer hops towards the surface, absence will be simultaneously filled by a vacancy from the underlying layer. If the vacancy diffusion coefficient is sufficiently large, the lowermost layer at the depth  $l$  will be supplied by a sufficient number of new vacancies and the flow  $J$  will not decrease with time. It is easy to show that when diffusion is limited, the inflow of vacancies after a while will stabilize and become constant although it will be lower. Therefore, we will use the value (8) for  $J$  henceforth.



**Fig. 5.** Flows of vacancies towards the surface ( $J$ ), resulting from exposure of particle beam.

If the surface is smooth, the flows are the same in all regions.

Now to study the stability of the surface, as it is done in [32], let us modify its shape along the  $x$ -axis with small sinusoidal perturbation of amplitude  $\gamma$  and frequency  $\omega$  (see. Figure 6). In this case, the surface shape  $Z(x)$  can be described by the equation:

$$Z(x) = z_0 + \gamma \sin(\omega x). \quad (9)$$

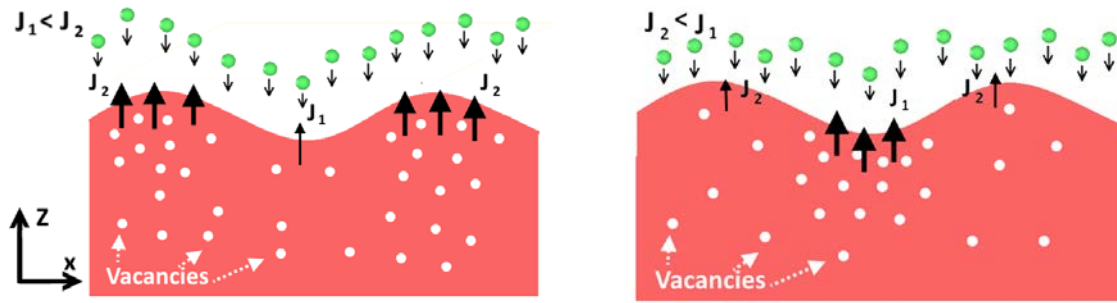
Such change in geometry, as it was shown in [30,32,34], affects the local stress  $\sigma$  near the surface:

$$\sigma|_{z_0+\gamma\sin(\omega x)} = \sigma_0 - 2\sigma_0\omega\gamma\sin(\omega x).$$

According to [3], such stress inhomogeneity will lead to change in vacancy concentration in the subsurface region, which depends on magnitude of the mechanical stresses and is given by:

$$n(x) = n_0 \left( 1 + \frac{\sigma\Omega}{kT} \right) = n_0 \left( 1 + \frac{[\sigma_0 - 2\sigma_0\omega\gamma\sin(\omega x)]\Omega}{kT} \right), \quad (10)$$

where  $\Omega = a^3$  is the volume occupied by a vacancy (or atom). Note that we considered tensile stress as positive. Thus, there may be a situation, shown in Figure 6. Depending on the sign of the stress, the increased concentration of vacancies will be either under the "hills" (Fig. 6a), or under the "valleys" (Fig. 6b)



**Fig. 6.** Surface of the crystal with a small sinusoidal perturbation of frequency  $\omega$ . Depending on the sign of mechanical stress vacancies may prevail near "hills" (a), or near "valleys" (b), and thus, flows of vacancies towards the surface will be maximal exactly in these areas.

According to the expression (8), the flow of vacancies towards the surface  $J(x)$  by means of the considered mechanism will be proportional to their local concentration  $n(x)$ . Substituting (10) into (8) yields the final expression for  $J(x)$  in various regions:

$$J(x) = Qpn_0 \left( 1 - \frac{[\sigma_0 - 2\sigma_0\omega\gamma\sin(\omega x)]\Omega}{kT} \right) \Omega. \quad (11)$$

The expression (11) contains full flow of vacancies towards the surface. Permanent part of it does not depend on  $x$ , and is responsible for the reduction in the overall size of the sample along the axis normal to the surface. But as the volume of the sample remains the same, it will increase in size along two other dimensions because of vacancy movement.

One can calculate change rate of the amplitude of the introduced sinusoidal perturbation from (11):

$$\frac{d\gamma}{dt} \sin(\omega x) = -\Omega J = Qpn_0 \left( \frac{2\sigma_0\omega\gamma\sin(\omega x)}{kT} \right) \Omega^3.$$

Therefore, in case of tensile stress ( $\sigma_0 > 0$ ) when vacancy concentration is higher near the "valleys", the impact of the beam of particles will lead to surface destruction near "valleys" and deepening faster than near "hills" resulting in increase in the perturbation amplitude. In case of compressive stress ( $\sigma_0 < 0$ ) maximal concentration of vacancies is observed near "hills", and the impact of the beam, on the contrary, will stabilize the flat surface, since the rate of surface destruction and deepening around "hills" will be higher.

Let us find a criterion of surface stability with respect to shape perturbations (9). We assume that the main factor, stabilizing the shape is the surface diffusion of adatoms [35]. Their concentration on the curved surface can be written according to the Gibbs-Thomson condition as:

$$C = C_0 \left( 1 + \frac{\theta\Omega}{kT} \omega^2 \gamma \sin(\omega x) \right),$$



where  $C_0$  is equilibrium concentration of adatoms on a flat surface, and  $\theta$  is surface tension. Heterogeneity in concentrations in different regions of the surface will lead to diffusion flux of adatoms  $J_D$  from the "hills" towards the "valleys", thereby leveling the surface. The rate of decrease in the perturbation amplitude via considered mechanism can be calculated as [30]:

$$\frac{d\gamma}{dt} \sin(\omega x) = -\Omega \frac{dJ_D}{dx} = -D\Omega \frac{\partial^2 C}{\partial^2 x} = -\frac{D\Omega^2 C_0 \theta}{kT} \omega^4 \gamma \sin(\omega x).$$

The total change rate of the amplitude  $\gamma$  consists of two parts corresponding to the surface diffusion of adatoms and to the flow of vacancies from the bulk crystal:

$$\frac{d\gamma}{dt} \sin(\omega x) = -\Omega J - \Omega \frac{dJ_D}{dx} = Qpn_0 \left( \frac{2\sigma_0 \omega \gamma \sin(\omega x)}{kT} \right) \Omega^3 - \frac{D\Omega^2 C_0 \theta}{kT} \omega^4 \gamma \sin(\omega x),$$

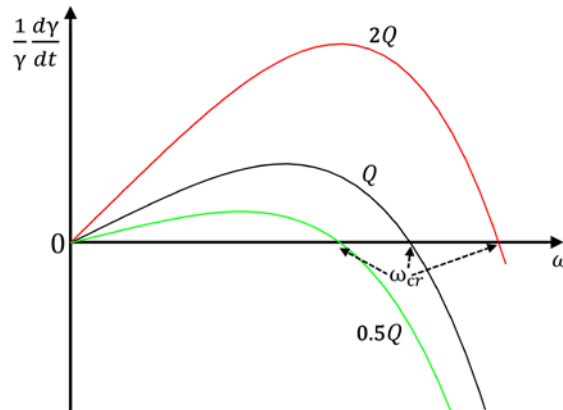
or:

$$\frac{1}{\gamma} \frac{d\gamma}{dt} = \frac{\Omega^2}{kT} \omega [2\sigma_0 \Omega Q p n_0 - D C_0 \theta \omega^3]. \quad (12)$$

Equation (12) implies that the surface is resistant to small perturbations (any perturbation will decay) when the expression in the parentheses is negative. It is easy to calculate critical perturbation frequency that is given by:

$$\omega_{cr} = \sqrt[3]{\frac{2\sigma_0 \Omega Q p n_0}{D C_0 \theta}}.$$

Any perturbation of a spatial frequency below  $\omega_{cr}$  will grow over time and the surface will change its shape. Note that  $\omega_{cr}$  frequency can be controlled via changing the parameters of the particle beam (energy, intensity), and thus, the rate of phonon generation  $Q$ . Figure 7 shows relative growth rate of perturbation at different values of  $Q$ .



**Fig. 7.** Dependence of the relative growth rate of amplitude of the perturbation on its spatial frequency for different  $Q$ . If the perturbation has a frequency less than  $\omega_{cr}$ , it will grow over time.

It should be noted that there are many other processes leading to the development of instability, in particular related to vacancy movement in the mechanically strained crystal. However, they have already been investigated and relevant criteria of stability have been found [30], so these processes have not been considered in this paper. A peculiarity of the above proposed mechanism is the possibility to influence the system from outside via adjusting the beam parameters. By increasing or decreasing its intensity, one can control the critical frequency, and thereby change the characteristic wavelength of perturbations on the sample surface. However, since most mechanisms of roughness development on flat surface manifest mainly at low spatial frequencies and have their own critical frequencies, it is obviously possible to control the surface roughness using the impact of the beam of particles only at higher frequencies when other mechanisms do not work.

What happens when the mechanical stresses are negative, i.e. are compressed? From the expression (12) it follows that surface is always stable, and any small perturbation will decay. If we consider other mechanisms of instability development, it is easy to see that usually the amplitude of perturbation growth rate is proportional to the frequency raised to the first or higher powers [30, 32, 34], and is determined by the internal parameters of the system (coefficients of diffusion at a given temperature, equilibrium concentrations, etc.). According to the above proposed mechanism, the rate of growth depends on the frequency linearly. Therefore, via controlling the beam parameters, one can make a "force" that appears under the influence of the beam of particles and leads to decay of perturbation. Such a "force" can suspend growth of perturbations via other mechanisms, and thereby make the surface flat and stable even with respect to long-wave perturbations.

We should note that in the above proposed models, there is no principle difference, what exactly the source of the lattice vibrations arising at the surface is. It may be any low-energy particles: atoms, clusters, molecules of gas, etc. Although in the simulation via MD we considered a beam of neutral particles and purely mechanical interactions, we can assume that the phenomenon of drift of vacancies towards the surface may be observed in the case of any other particles with low energy capable anyhow to transmit momentum to the lattice, for example, photons.

## 5. Conclusions

We proposed a mechanism of change in morphology of the surface of crystalline solids under the influence of the local beam of low-energy particles, as well as under uniform illumination of the crystal surface. It has been shown that such change may be due to scattering of the lattice vibrations generated near the surface on the vacancies. This causes a drift of vacancies to the spot of the beam incidence. Two modes are showcased: ballistic and diffusion. Their differences are shown and time dependence of the rate of change of the surface profile is found. It is shown that the phonon mean free path  $l$  and some other characteristics of the process, for example, the values of  $Q$  and  $p$ , can be found from the analysis of this dependence. The discovered mechanism of morphology change is most effective when tensile stresses increasing the concentration of vacancies are applied to the crystal. The process of the roughness development on the surface of the elastically-strained crystal was investigated and it is shown that an arbitrary small perturbation of the surface may grow indefinitely under certain conditions because of the nonuniform flow of vacancies towards the surface. Instability appears at spatial frequencies below the critical  $\omega_{cr}$ , which is determined by intensity of phonon generation, concentration of vacancies, the magnitude and sign of mechanical stress, as well as other parameters of the system. It is shown that if the stresses are negative (compressive), vacancy drift reduces the roughness. This phenomenon can be used to suppress development of instability via other mechanisms even with respect to low-frequency perturbations.

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