ACCELERATION OF ATOMS DURING PHASE TRANSITIONS ON CRYSTAL SURFACES

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The paper explores a possibility of the coherent energy transfer from many adatoms initially in metastable states to a single accelerated adatom during a phase transition at the crystal surface. The acceleration occurs as a long chain of subsequent collisions with a single particle gaining momentum harvesting the energy of the transition of its predecessor in the row from the metastable to the stable state. The paper presents the analysis of the stability of the suggested system, simulation of the dynamics of accelerations, and the analysis of the limits imposed on the process by the defocusing effect.

1. Introduction

Energetic particles are used in order to accelerate the processes running in target materials, modify them, and, what is most important, stimulate those of them which require threshold energies. Therefore, obtaining fast particles is an important part of the human efforts in the study of the nature, as well as in the applications [1, 2]. Particle acceleration is usually associated with external electric fields. In order to be accelerated in an electric field, particles have to either possess a charge or a non-uniform charge distribution. A series of publications [3–5] suggested a mechanism of acceleration of atoms in a non-equilibrium system during its transition to the equilibrium state. The atoms can be neutral. A prerequisite for the acceleration is the existence of two energy minima for atomic positions along a certain direction in the crystal. The acceleration occurs when the atoms initially occupy positions with greater energy. Qualitatively, the considered acceleration effect can be presented as follows. Let us imagine a system, in which there are two potential minima for an atom in a certain direction, and let the atoms are situated initially in the upper minimum. Such a state is metastable, and the atoms would move in the course of time to the positions with smaller energy. Atoms can relax separately. However, as works [3–5] showed, the relaxation can occur in a coherent way so that the atoms along an atomic chain would undergo subsequent transitions transferring their energy to the next ones in the row. As the coherent relaxation, we will call such processes when the relaxation of one atom from the metastable state to the stable state stimulates the relaxation of the next atom as a result of the collision. Let one of the atoms acquire some energy (from an external source or fluctuationally) which is sufficient for overcoming the potential barrier and collide with a neighbor atom. As known, at the central collision of moving and stationary balls, the moving ball stops, and the stationary ball starts to move. If the first atom stops after the collision in the vicinity of the lower minimum (point A in Fig. 1), then it transfers the energy released at the relaxation to the second atom. As a result, the second atom accelerates. Further, such energy transfer of the energy released at the relaxation into the energy of the motion of the last atom in the chain occurs at every consequent collision. As the transition of each of the atoms from the high energy state to the low energy state is accompanied with some energy gain, these gains accumulate, and the energy transferred to the last atom in the chain can grow very strongly provided the number of subsequent collisions is sufficiently large.

Therefore, as a result of the consequent collisions, the acceleration of a single atom occurs. The above-presented considerations are qualitative. The real atoms cannot be considered as elastic balls. In addition, the colliding atoms are not free but move in the external potential which has formed the two-well potential. However, the analytic calculations performed in [3] and the computer simulation of the motion of a chain of atoms interacting with one another and affected by the external forces [4, 5] showed that such an acceleration exists.

The acceleration is facilitated by the phenomenon of focusing which is well known in radiation physics and confines the motion of atoms to a certain crystal direction, if their energy does not exceed a certain threshold value in the range of hundreds of eV.

The principal questions in this problem are as follows: 1) is the two-well potential along a crystal direction possible, 2) could the inverse population, when

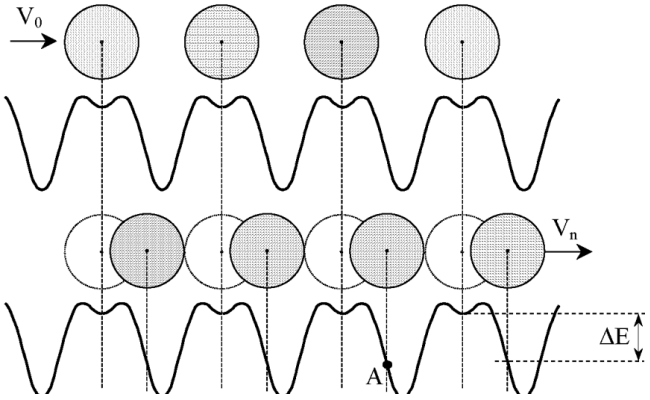

Fig. 1. Schematic illustration of the acceleration mechanism. At the top, the initial metastable state is shown. The bottom row shows the process during which each of the atoms in the chain is displaced prior to a collision to a position where its potential energy is smaller than the energy in the initial state. Accordingly, the next atom in the chain gains the same value of kinetic energy

atoms occupy the wells with the higher energy, occur, and 3) which is the largest energy the accelerated atom can acquire? Such an acceleration can occur during a structural phase transition in strongly strained crystals during the movement of a screw dislocation [3–6], as well as in a system with the "domino"-type photoinduced phase transition [7]. The term "acceleron" has been coined in works [3–5] to refer to the crystal state with a sequence of atomic collisions accelerating a single atom. The estimates of different mechanisms of energy loss at collisions [3–5] show that the energy of an acceleron can be as high as one hundred eV.

The suggested mechanism differs from the other known mechanisms. The acceleration of this kind can occur during the relaxation of a non-equilibrium state. As the energy of the accelerated particle is much greater than kT, accelerons could be one of the reasons for a number of anomalous phenomena: the emission of electromagnetic waves in the UV and X-ray spectral ranges as a result of atomic excitations at collisions, the increase in the probability of low-threshold nuclear reactions, *etc.*

The previous works presented the results of one-dimensional simulations of the acceleron dynamics, i.e. only one chain of atoms was simulated. In this work, we performed the simulation of a two-dimensional system, namely the layer of atoms, by taking the temperature effects into account. In this case, the model considers the dynamics of atoms which can be in two energy minima and allows one to simulate the energy dissipation from the chain of collisions along the perpendicular direction.

As shown in work [4], one of the systems where accelerons can appear is a crystal in a state preceding the phase transition where the inversion of the population of crystal sites could arise at the boundary between different phases. The fact that the growing new-phase nucleus has shape close to a spherical one in most cases presents a difficulty for the creation of accelerons, since no inverse population arises along a certain row, which is important for the suggested mechanism. This is the reason for the simulation of the atomic acceleration at the crystal surface. There is a great variety of structural phase transitions in systems of adatoms on the crystal surface [8–10]. Some of these phase transitions can be suitable for the purpose of creating the systems with long rows of atoms in metastable positions. This paper presents a simulation of the acceleration process happening on the flat surface during a surface phase transition.

2. Model

We consider a system of adatoms on a crystal surface, assuming that they can form two different lattices comprising two phases, one of which is stable and the other is metastable. Our purpose is to study the dynamics of a phase transition, during which an acceleron an appear. In the first approximation, we will perform simulations in two dimensions. Simulations in 3D allowing atoms to move in the direction perpendicular to the plane were performed as well and showed no significant difference in results.

In the proposed model, the adatoms above the crystal surface interact with one another, as well as are affected by a potential imposed by the surface. The total potential energy is, thus, given by the expression

$$U(\{\mathbf{r}\}) = \sum_i U_{\text{ex}}(\mathbf{r}_i) + \frac{1}{2}\sum_{i\neq j} U_{\text{in}}(\mathbf{r}_i - \mathbf{r}_j), \qquad (1)$$

where $\mathbf{r}_i$ are coordinates of the i-th atom, U_{in} is the potential of the interatomic interaction, and U_{ex} is the external periodic potential created by atoms of the substrate.

We have chosen the Lennard-Jones potential for the interaction between the atoms:

$$U_{\text{in}} = U_0\left(-\frac{r_0^6}{r^6} + \frac{r_0^{12}}{2\,r^{12}}.\right) \qquad (2)$$

In what follows, we use such dimensionless units that $U_0 = 1$ and $r_0 = 1$. The length units are such that the Lennard-Jones potential has a minimum at $r = 1$. For

the realistic systems, the unit of energy may vary in the range of 0.5÷3 eV.

When the interaction with the surface is not taken into account, a two-dimensional system of adatoms interacting via a spherically symmetric potential would form a hexagonal lattice. We assume that the surface imposes an additional field on adatoms in such a manner to prevent this possibility. The external potential is chosen to define a square grid and taken in the form

$$U_{\rm ex}(x,y) = U_e \left(-\cos\frac{4\pi x}{a} - \cos\frac{4\pi y}{a} - \frac{1}{4}\cos\frac{8\pi x}{a} - \right.$$

$$\left. -\frac{1}{4}\cos\frac{8\pi y}{a} \right). \qquad (3)$$

Two last cosines in the potential do not create additional minima but help to make the wells narrower and the barriers smoother.

We consider a system, in which the adatoms occupy a quarter of the potential wells defined by the grid (every second minimum in each direction). The coefficient U_e which determines the interaction of adatoms with the surface is considered to be small, while, at the same time, strong enough to prevent adatoms from forming a hexagonal lattice.

Thus, when the atoms occupy every second site of the grid along each row, one can construct two types of lattices shown in Fig. 2: a square lattice and a lattice with a shifted row which could be classified as a rectangular centered one. We consider a phase transition between those two lattices. Each of them has the same energy in the external potential of the substrate, but their energies differ due to the interatomic interaction. In the lattice with shifted rows, the distance between atoms is larger, but, at the same time, the number of the closest neighbors increases. The balance between those factors determines which of the lattices is more stable depending on the grid period a. Calculations show that the square lattice becomes more stable at $a > 1.05825$ in units of r_0. For a smaller period of the external potential, the lattice with shifted rows is energetically preferable.

Without the stabilizing interaction with the substrate, a two-dimensional system of spherical atoms would form a hexagonal close-packed lattice with a symmetry different from both proposed arrangements. This fact is a source of a possible instability of the system.

We suggest to study mechanisms of the phase transition from the initial square lattice to the lattice

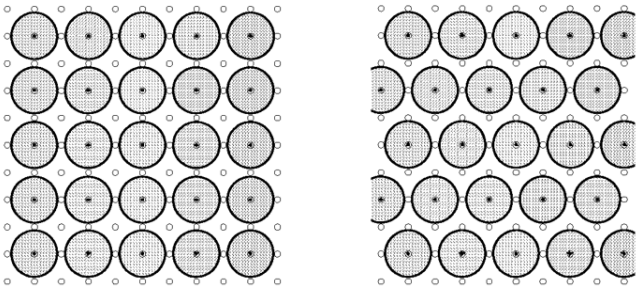

Fig. 2. Two types of a lattice which can be formed by adatoms above the grid defined by the surface: a square lattice is on the left and the lattice with shifted rows is on the right

with shifted rows. We assume that the initial square lattice of adatoms has been formed, for example, at a higher temperature when the lattice of the substrate is more spacious. At a decrease in the temperature or as a result of the hydrostatic compression, the period of the substrate-imposed potential can decrease and the system of adatoms would find itself in a metastable state. This metastable state is chosen as the initial state in the modeling.

3. Analysis of Stability

The arrangement of adatoms in the surface layer is determined both by the interaction between the adatoms and the interaction with the substrate, whose structure is assumed to be fixed. We consider the case where the adatoms occupy the sites determined by the substrate potential. The stability of the arrangement of atoms is analyzed both for the square lattice and the lattice with shifted rows. The criterion of the stability of the system is the condition that the matrix of the second derivatives of the potential with respect to a displacement of atoms from the equilibrium position would be positively determined.

Coordinates of the i-th adatom can be written in the form $\mathbf{r}_i^p = \mathbf{r}_i^0 + \mathbf{r}_i$, where $\mathbf{r}_i^0$ are the coordinates of the lattice sites and $\mathbf{r}_i$ are small displacements which can be presented in the form $\mathbf{r}_i = \sum_{\mathbf{k}} \mathbf{r}_{\mathbf{k}} \exp(i\mathbf{k}\cdot\mathbf{r}_i^0)$.

We obtain the expansion of the potential in Eq. (3) in a series of displacements after some straightforward transformations

$$U(\{\mathbf{r}_i\}) = \sum_i U_{\rm ex}(\mathbf{r}_i^p) + \frac{1}{2}\sum_{i\neq j} U_{\rm in}(\mathbf{r}_i^p - \mathbf{r}_j^p) = U_0 \qquad (4)$$

$$+N\sum_{\mathbf{k}} |x_{\mathbf{k}}|^2 \left(\frac{16\pi^2 U_e}{a^2} + \sum_{i\neq 0} \frac{\partial^2 U_{\rm in}(\mathbf{r}_i^0)}{\partial x^2} \sin^2\frac{\mathbf{k}\mathbf{r}_i^0}{2} \right) \qquad (5)$$

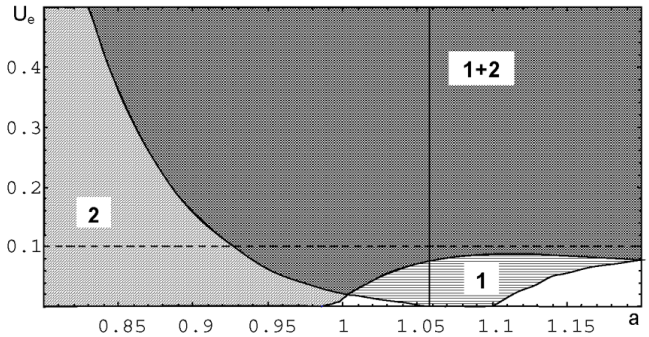

Fig. 3. Regions of stability of two types of lattices versus the surface grid period a and the value of the surface potential U_e. The region of stability of the square lattice is denoted as 1, the same for the lattice with shifted rows is denoted as 2. In the (1+2)-region of parameters, both lattices are stable

$$+N\sum_{\mathbf{k}}|y_{\mathbf{k}}|^2\left(\frac{16\pi^2U_e}{a^2}+\sum_{i\neq 0}\frac{\partial^2U_{\rm in}(\mathbf{r}_i^0)}{\partial y^2}\sin^2\frac{\mathbf{kr}_i^0}{2}\right). \quad (6)$$

The factors at $|x_{\mathbf{k}}|^2$ and $|y_{\mathbf{k}}|^2$ should be positive for all values of $\mathbf{k}$ if the atomic positions in the sites are minima.

Figure 3 shows the diagram of stability of the square lattice and the lattice with shifted rows depending on the period of the surface grid a (x-axis) and the external potential amplitude U_e (y-axis). To the left from the vertical line at $a = 1.05825$, the lattice with shifted rows has a smaller energy, while, to the right from that line, the square lattice has a smaller energy.

Numerical calculations show that the square lattice is locally stable even without external potential at $1.06923 < a < 1.09512$. For example, at $U_e = 0.1$ in units of U_0, the square lattice is stable, when $a > 0.92607$.

4. Metastable Atomic Positions

The stability analysis shows that, in a certain region of parameters, there exist two possible states for the lattice of adatoms, one of which is stable and the other is metastable. In the metastable lattice, a row of atoms sandwiched between its neighbors has two local minima separated by the period of the grid (the half period of the lattice of adatoms) which correspond to the different lattices. A transition of a row from one minimum to another one is a structural phase transition.

Figure 4 shows a variation of the potential energy of a row depending on its position. This energy is a sum of the energies of interaction with the substrate and other adatoms. The difference of the depths of the potential

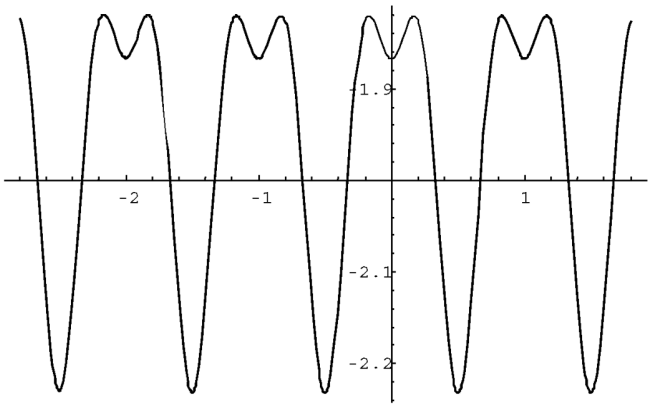

Fig. 4. Potential for the atoms of a row as a function of a displacement showing the stable and metastable positions. The amplitude of the surface potential $U_e = 0.1$. The grid lattice period is 0.96

minima determines the energy which could be released when a row shifts by a grid period and, thus, is important for the acceleron formation.

As was mentioned in Introduction, the mechanism is related to subsequent collisions of atoms and their transfer from the top well to the lower potential minimum.

The mechanism of acceleron creation is described qualitatively in Inroduction. After acquiring a sufficient kinetic energy from a collision with its neighbor, an atom initially localized in the top well overcomes a low potential barrier and moves toward a lower potential minimum until the repulsion from the next atom in the row is sufficiently strong. Upon a new collision, the atom under consideration stops, giving away its energy. Thus, the incident atom stops, and the next atom moves away with the energy increased by the relaxation energy of the atom. This energy gain depends on the point, where the atom under consideration stops. If the atom stops close to the well bottom, the energy gain is large, and when it stops close to the highest point of the potential barrier, the energy gain is small. The particles can even lose energy if they are stopped at the top of the potential barrier.

5. Modeling and Results

Molecular dynamic modeling was performed for the 250×8 strip of atoms initially located on the square grid with the period $a = 0.96$ and for the external

potential amplitude $U_e = 0.1$. The simulation software numerically solved the system of Newton equations

$$m\frac{d^2\mathbf{r}_i}{dt^2} = -\nabla_i U(\{\mathbf{r}\}), \tag{7}$$

where $U(\{\mathbf{r}\})$ is given by Eq. (1), and m is the mass of an atom.

As mentioned above, in order to form an acceleron, an atom has to overcome the potential barrier. This can happen either due to an impact of the external origin or due to thermal fluctuations. In this paper, the former situation is considered. We studied the region of temperatures sufficiently low in order that the transitions of atoms from the upper to the lower well due to thermal fluctuations be extremely rare. Therefore, if the atoms are initially in the vicinity of the upper wells, they will stay there indefinitely long. The temperature effect in the initial system is reduced to the equilibrium vibrations within the metastable state.

For the simulation, we initially assigned small Gauss distributed velocities with some small mean energy to all atoms, and the system was equilibrated for a certain period of time. During the equilibration, the atomic motion acquired a temperature defined by the chosen mean energy, and all correlations were properly set. After that, an atom at some lattice site was assigned a significant velocity along the x-axis.

The program followed the atoms with the largest velocity, and when its distance from the end of the strip was less than 150 lattice periods, the modeled region moved forward by a period: new atoms were added at the end of the strip while the atoms at the beginning of the strip were thrown away. By using this procedure, we were able to follow the acceleration for a significant period of time by running the dynamics of a small number of atoms. As the acceleron is faster than other oscillations in the system, the dynamics of the atoms left behind does not affect its propagation while the added atoms were far enough to justify the addition at the fixed position in the lattice sites. The number of atoms between the high-velocity atom and the boundary of the simulation window allows us to expect that the thermal equilibrium is always set in the region of the acceleron prior to its arrival.

First, we simulated the acceleration at a practically zero temperature when the energy of atomic vibrations was 10^{-5} in dimensionless units. Figure 5 shows the time dependence of the velocity of every 50-th atom along the acceleron path. As the acceleron propagates, the velocity of each next atom increases due to the coherent adsorption of the energy released at the relaxation. For

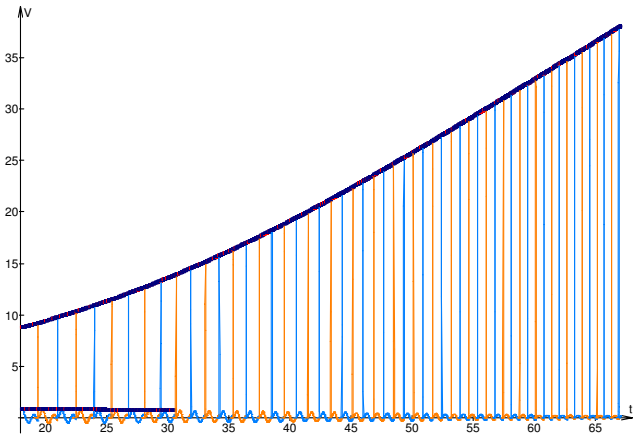

Fig. 5. Time dependence of the velocity of each 50-th atom in the collision chain in the simulation. The plot clearly shows the gradual acceleration of the adatoms in the chain

faster atoms, the time interval between the peaks decreases. One can see that the energy accumulates in the form of the kinetic energy of a single atom.

As the acceleron propagates along the crystal, the atoms left behind shift by a period of the substrate grid. In this manner, the lattice behind the acceleron changes its symmetry. During the time of simulation, the other rows were not affected by the transition, and the remaining part of the released energy (which was not accumulated by the accelerated atom) dissipated.

The analysis of the time dependence of the positions of atoms left behind the acceleron shows that the faster they move, the closer to the well bottom each atom stops. Therefore, the energy transferred further along the row is larger, and the amplitude of the subsequent vibrations is smaller. The efficiency of the acceleration grows with each collision.

6. Defocusing

There are several factors limiting the energy of the accelerated atom: structural defects, impurities, thermal oscillations, and defocusing. Their effects have been estimated in [4,5]. They can be decreased by a choice of a more perfect system and by lowering the temperature. However, the defocusing cannot be suppressed or eliminated. We have carried out its modeling. The propagation of an acceleron requires the presence of straight rows of atoms. The accelerating propagation occurs along this row. Moving at an angle to this direction, an atom experiences a non-central collision. In this case, its kinetic energy cannot be transferred to

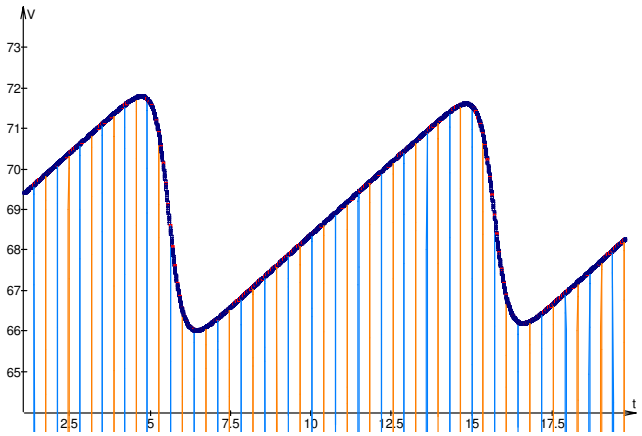

Fig. 6. Defocusing effect. The velocity of each 50-th atom in the collision chain is shown as a function of time. Defocusing leads to a decrease of the kinetic energy of the fastest atom. The acceleration process picks up again after the velocity decreases below the level of defocusing

the next atom in the chain. However, at small energies, there exists the well-known focusing effect: after each subsequent collision, the deviation of the direction of the atomic motion from the line formed by the atomic row decreases (see [11]). According to calculations, the focusing effect holds up to the energy of several hundred eV, dissapearing at larger energies. When the accelerated particles reach that value of energy, the random deviations from the direction of propagation would tend to increase.

Results of the modeling of the defocusing effect are shown in Fig. 6. The simulation has been performed in the vicinity of the threshold velocity for the thermal vibration of order of 10^{-3}. For the chosen parameters, the threshold value of the velocity in dimensionless units is 69. In order to reach that velocity, the atoms in the row have to experience approximately 1000 collisions. After that, the energy losses due to the defocusing effect prevail, and the propagation of accelerons slows down. Further simulations show that, in this particular model system, the acceleration starts anew after the energy of the fastest particle becomes sufficiently small.

7. Scattering on Thermal Vibrations

An increase of the amplitude of thermal vibrations affects the scenario of events in such way that the acceleration slows down. In order to evaluate this effect, we performed simulations at different temperatures. The results are summarized in Fig. 7.

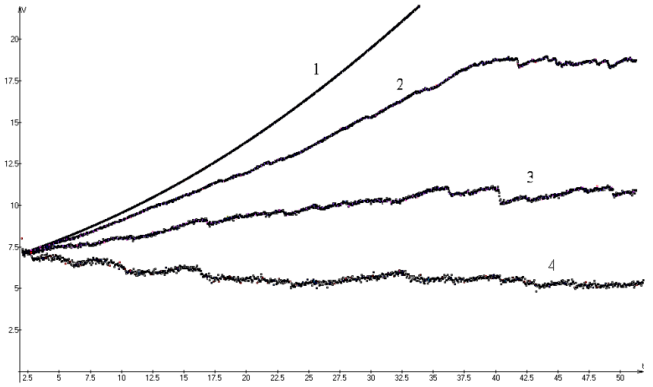

Fig. 7. The acceleration curves for simulations performed for different temperatures of the system. *1*: T=10^{-5}; *2*: T=0.001; *3*: T=0.0033; *4*: T=0.01

At non-zero temperatures, one can see a decrease of the acceleration rate due to the energy dissipation on thermal vibrations. In addition, occasional greater energy losses are seen, which is believed to be the dissipation on so big thermal fluctuations that the focusing needs about a dozen of collisions to reset the one-dimensionality of the acceleron.

Each temperature sets a limit for the highest energy the atom may acquire in the collision chain. This is clearly seen from curve *2*. If the initial energy exceeds this maximum, the atoms slow down, as it seen from curve *4*.

Let us assume for the estimates that the energy unit U_0 = 2 eV. Then the analysis of the curves in Fig. 7 shows the highest energy an acceleron may acquire at a temperature of 150 K is 30±5 eV. The acceleration may occur at this and higher temperatures if the initial energy of the acceleron is lower than the limit.

The mechanism of acceleration at low energies is more complicated. It will be considered in the next section. The determination of the temperature limit, at which the coherent atomic acceleration can occur, requires to consider the case where the initial dropping of an atom from the high-energy position to the lower energy well occurs fluctuationally. Such a study is beyond the scope of the present paper.

8. Acceleration at Low Energies

If the energy obtained by the first particles in the chain of accelerations is sufficient to overcome the potential barrier but is not sufficient for the transition to the next deeper potential well, i.e., if the atom stops at the slope higher than its initial position in the shallower well,

the energy communicated to the next atom in the row at the collision will be less than the kinetic energy of the initial atom. In this case, the propagating chain of collisions initially slows down. However, it leaves behind a number of high-energy atoms stopped at the slopes. The relaxation of these atoms occurs in a coherent way as well. The particles continue to move in the same direction at the acceleron speeding up. As a result, a second acceleron is formed. As the atom at the head of the chain of collisions slows down and the atoms left behind gain velocity, the second acceleron approaches the first one and pushes it forward increasing the energy. This process is illustrated by the time dependence of the velocities of the fastest atoms along the row shown in Fig. 8. This shunting can occur several times till the energy of the atom at the head of the collision chain at the point where it stops is smaller than the energy of the shallow well bottom. At this point, the front atom starts accelerating and the remaining energy of the left behind atoms is not sufficient to support the second acceleron.

As a result, for a short chain of acceleration, two fast particles can leave the system instead of a single accelerated particle. Simulations for a long finite strip of atoms carried out in 2D and 3D cases confirmed this conclusion. However, the energy of accelerated particles was not large.

At some values of the parameters, the point, where the first of two accelerons escapes the second one, has never been reached. In these cases, the second acceleron periodically reaches the first and pushes it, but the acceleration to a greater velocity does not occur, and the energy of the phase transition is dissipated incoherently. As a result, two moderately accelerated particles leave the system.

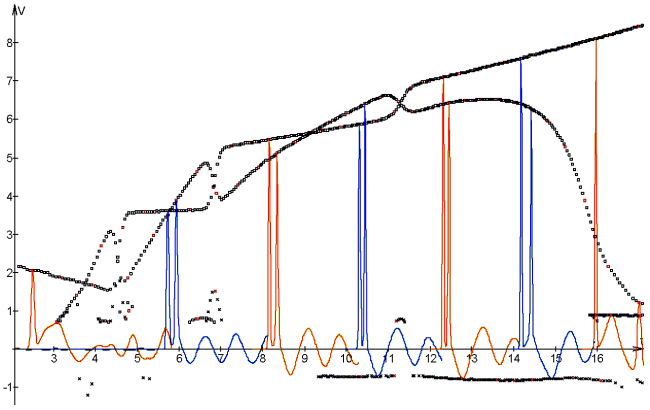

Fig. 8. Acceleration at the initial stage showing two fast atoms propagating along the row. The second accelerated atom moves faster than the leading atom in the collision chain. Eventually, it approaches the leading atom and pushes it forward. The process lasts till the leading atom gains enough energy to undergo collisions in the position when the further gain of energy is possible. After that, the second fast atom obtains less energy in the collisions and eventually disappears

9. Conclusions

The paper presents the results of the molecular dynamics simulation of the atomic acceleration as one of the mechanisms of energy relaxation at surface phase transitions. The analysis of the requirements to a system, in which such acceleration is possible, has been performed. The possibility of the propagation of two accelerated atoms along a row is discovered by the simulation. In the studied model of acceleration, one of the atoms on the initial grid was given a certain energy in order to overcome the potential barrier between the atoms. Under real conditions, such an energy can be communicated to an atom by the external low-energy beam of particles or as a result of fluctuations. The acceleration in a fluctuating system and the energy distribution of accelerated atoms require further studies that are planned in the continuation of the current research.

So far the accelerons were not observed experimentally. However, no experiments that would intentionally look for them were performed. At the same time, the fast moving atoms in crystals can manifest themselves in the appearance of processes, whose triggering requires the energy significantly exceeding kT. Some anomalous phenomena in crystals have not found a satisfactory explanation, whereas accelerons can play a certain role in them. A number of such phenomena have been analyzed in [12]. Among them are the visible optical emission arising at the ultrasonic irradiation of semiconductors, cold nuclear synthesis, anomalous mass transfer, *etc.*

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МОДЕЛЬ ПРИСКОРЕННЯ АТОМІВ ПРИ ФАЗОВИХ ПЕРЕТВОРЕННЯХ ПОВЕРХНІ В КРИСТАЛАХ

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Р е з ю м е

В роботі досліджено можливість когерентної передачі енергії багатьох атомів, що початково перебувають в метастабільному стані, одному прискореному атому при фазовому переході на кристалічній поверхні. Прискорення відбувається в результаті довгої низки послідовних зіткнень, за яких одна частинка в ряду набирає швидкість, збираючи енергію, яка виділяється при переході всіх попередніх із метастабільного в стабільний стан. В роботі проведено аналіз стабільності запропонованої системи, чисельне моделювання динаміки прискорення і аналіз обмежень, які накладає на цей процес дефокусування. Показано, що нейтральна частинка може бути прискорена запропонованим способом до енергій порядку декількох сотень еВ.