Influence of Radiation on the Interatomic Interaction in Metals

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Abstract – The interatomic potential for the cases when ionization and excitation of the free electron gas took place was investigated for aluminum as a sample. The Heine-Abarenkov-Animalu model potential form factors was employed. The form factor parameters of ionized atoms was determined on the base of the quantum defect method using the atomic-spectroscopy data. The potential of interatomic interaction for different charged states and the equation of the matter states with different degree of ionization were determined. The potential function is calculated for case when excitation of the free electron gas takes place

1. Introduction

Low-energy ion beams and plasma have found wide application in the scientific researches and the practical purposes They are used in accelerators of the charged particles, in ionic – plasma technological installations, in the equipment for radiating tests, etc.

Bombardment of a surface of metals by fast ions and atoms is accompanied by the physical processes connected with transformation and transfer of energy of falling particles to the material of the target.

Presence in the metal of two interconnected subsystems, ionic and electronic, leads to that correct consideration of processes dissipation energy is the complicated problem.

In – the first, interaction of plasma and ionic beams with ionic and electronic subsystems occurs under various laws, in the second, there is a redistribution of energy from one subsystem to another during influence of the radiation.

The processes of the ion beam energy relaxation in metals are necessary to study in view of redistribution of energy between ionic and electronic subsystems.

2. Ways of the energy relaxation

In Fig. 1 the basic physical processes connected with redistribution of energy in metal during influence of streams of plasma and low-energy ion beams are presented.

Let's consider briefly each of these processes separately. We shall begin with influence on the ionic subsystem.

Nuclear braking is caused by coulomb interaction of atomic nucleus of irradiated substance with the moving ion. It causes formation of initially beaten out atoms and radiation defects.

Characteristic time of existence of the atomic collisions cascade makes approximately $10^{-11} \dots 10^{-12}$ s.

The size of the cascade and the existence time depend on energy of the bombarding ion. The atomic dispersion of the target occurs as a result of the cascade processes near to the surface.

After a while on a place of the atomic collisions cascade the thermal peak is formed. It represents the atomic structure possessing a heat. From the thermal peak there is the atoms evaporation if it is near to target surface. Characteristic time of existence of the thermal peak makes approximately $10^{-11} \dots 10^{-12}$ s. [1].

The diffusion processes intensively occur in the field of the thermal peak. The reason of it consists in a heat of the thermal peak substance and in greater gradients of temperature and pressure. These phenomena lead to significant change of structure and properties of the irradiated substance.

A plenty of the ionized atoms is formed in the field of the track of the high-energy ion. The potentials of interatomic interaction change between the ionized atoms. The atoms start to make a start from each other. This phenomenon is capable to cause the cascade processes, to lead to dispersion the target atoms, to intensify the diffusion processes.

The recombination of the ionized atoms occurs, basically, two ways – Auger recombination and radiating recombination.

The radiating recombination it is accompanied by absorption of one electron from the zone of conductivity and radiation of the x-ray photon or the optical photon. The characteristic time of the radiating recombination makes not less than 10^{-14} s. [2]. Here the phenomenon of the capture of radiation takes place. The photon is absorbed by other ions with the subsequent reradiation.

Auger recombination occurs to participation of two electrons from a zone of conductivity. In this case one electron is grasped by the ion, and the second carries away the kinetic energy. The characteristic time of the Auger recombination makes approximately $10^{-15} \dots 10^{-14}$ s. This energy will be transformed to the thermal energy of the target.

Let's consider the basic processes proceeding in the electronic subsystem.

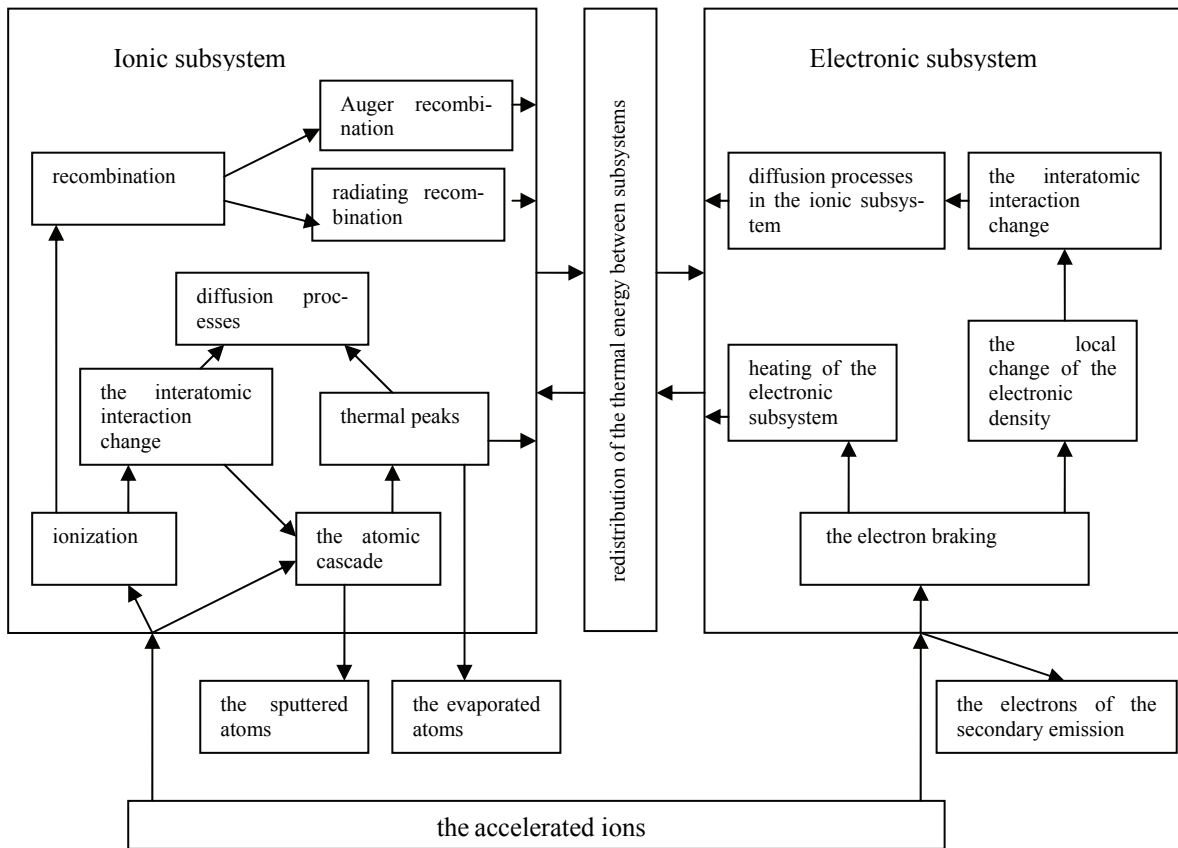Bombardment of the target surface by the accelerated ions causes secondary electron emission.

Fig. 1. The basic physical processes connected with redistribution of energy in metal during influence of streams of plasma and low-energy ion beams

The secondary electron emission it is caused Auger recombination of the conductivity electrons on the accelerated ions. The characteristic time of the surface Auger recombination makes approximately $10^{-15}\ldots10^{-16}$ s [3].

The accelerated ions are braked by free electron gas. There is a warming up of the electronic subsystem and local change of the electron density.

The heat is redistributed between electronic and ionic subsystems. Local change of electron density leads to change of interatomic interaction. This phenomenon strengthens diffusion processes in the ionic subsystem.

All the considered phenomena are interconnected among themselves. Therefore we have tried to consider these phenomena in common.

3. Interatomic interaction

The interatomic potential for the case when ionization took place was investigated for aluminum as a sample. The Heine-Abarenkov-Animalu model potential form factors was employed. The form factor parameters of ionized atoms was determined on the base of the quantum defect method using the atomic-spectroscopy data [4].

Fig. 1 represents the potential of interatomic interaction for different charged states in aluminum which were estimated using the above data. Calculation was done for a situation when the ionized atom concentration is small and consequently the conduction electron concentration does not differ from an usual one.
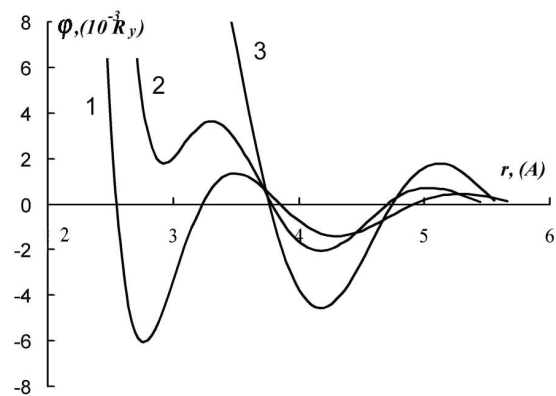

Fig. 2. Interatomic potential: $1 - Al^{3+}$ and Al^{3+}; $2 - Al^{4+}$ and Al^{3+}; $3 - Al^{4+}$ and Al^{4+}

This figure shows that ionization leads to the strong decrease in the depth of the first minimum of the potential function corresponding to the distance area between the nearest neighbors for three- or four-charged ions. Moreover, for the pair of particles with

four charges the first minimum disappears absolutely. Atoms fall to the repulsion branch of interaction potential. As a result, the crystal lattice changes to the state of nonequilibrium [5, 6].

Shielding properties of the electrons conductivity are defined by their concentration. In Fig. 3 the potentials of interatomic interaction for a case when concentration of the electrons conductivity is more than normal on 30 % (an impulse electrons on Fermi's surface on 10 % more normal) are shown
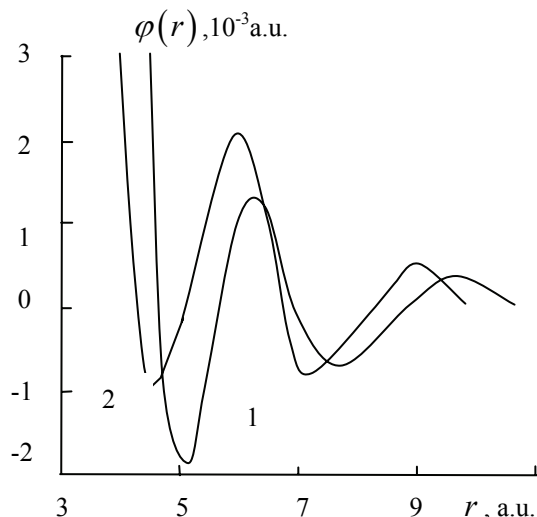

Fig. 3. Interatomic potential for Al: 1 – normal condition; 2 – 10 % excess of an impulse of the electrons conductivity above Fermi's

Local growth of the electrons concentration can arise in the field of a track of the fast charged particle and to lead to "softening" of a crystal lattice [7].

On the basis of the similar potentials of interatomic interactions, applying the method of molecular dynamics, we modeled the dispersion of aluminum surface within the track of charged particles. It was shown that ionization greatly affects the dispersion process of surfaces of metals.

The most part of the ionized atoms in the field of the track gets high speeds and leaves the surface during order 10^{-13} s. It is commensurable with duration of existence of the ionized conditions in metal [8].

4. Diffusion process

There are greater gradients of temperature and thermomechanical pressure at pulse strong influence of the charged particles on the metal surface.

The diffusion processes in aluminium at presence of the gradient of temperature were modelled by the molecular dynamics method.

Dependences of the thermodiffision ratio k_T and the diffusion stream (normalized on the unit gradient of temperature ΔT) $k_T D/T$ from temperature T have been calculated.

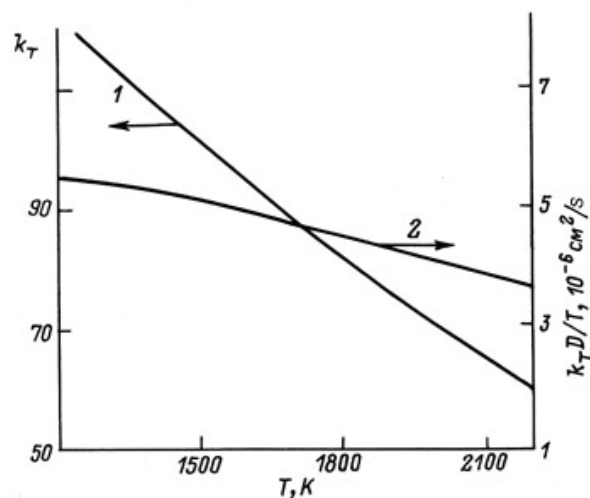These dependences are presented in Fig. 4.

Fig. 4. Thermodiffision ratio (1) and diffusion stream (2) as function of the temperature

Decrease k_T with growth T is result of stochastic character of the atoms moving. Movement of atoms in the field ΔT is small in comparison with casual wanderings at heats [9].

It has been shown, that settlement concentration structures will well be coordinated with experimental one if to apply the thermodiffision ratio from Fig. 4.
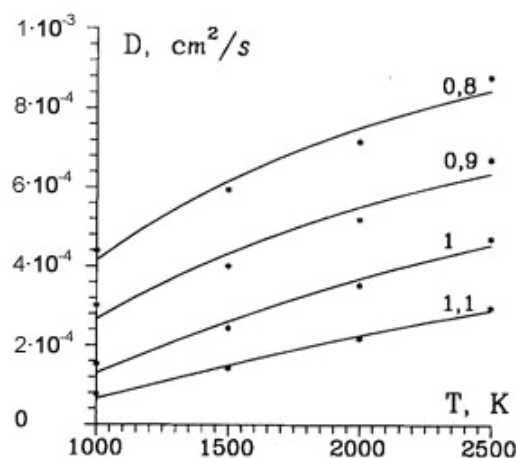

Fig. 4. Diffusion constant of liquid aluminium as function of the temperature and the density

Figures on curves it are the ratio of local density to normal. Asterisks it are the results received by means molecular dynamics method. Continuous lines it are results received by means of approximation by the least – squares method of Arrenius expression [10].

It has been shown, that reduction of the substance density causes the big increase of the atoms mobility. It is caused, basically, reduction of the diffusion activation energy.

Therefore, on the basis of the pseudopotential approach of the previously obtained materials using

aluminium as an example, we constructed the equations of conditions of metals, taking into account the ionized conditions.

However, the molecular-dynamic dispersion modeling in many cases is qualitative. For the more thorough investigation of destruction processes of surfaces we should solve the equation of thermal elasticity, where in its turn we should know the equation of substance condition [8].

5. Equation of matter state

While studying the radiation-stimulated processes it is necessary to learn out not only the interatomic coupling potential, but the consistent relations considering the ionized particles, as well. Such relations can be provided on the basis of binding energy.

This one for the secondary model

$$E(\Omega) = E_e^{(0)} + E_e^{(1)} + E_e^{(2)} + E_i. \qquad (1)$$

Where Ω – atomic volume, $E_e^{(0)}$ – the energy of homoheneous electron gas, including the kinetic, exchange and correlative energy of conduction electrons, $E_e^{(1)}$ – the energy, caused by the fact that the ions are not the points and have some dimensions, $E_e^{(2)}$ – energy of zonal structure, E_i – Evald energy.

Static component of pressure- can be defined by equation

$$P_{st}(\Omega) = -\frac{dE}{d\Omega}. \qquad (2)$$

The contribution caused by harmonic phonon pressure and zero oscillation energy has been negligible.

The registration of differently ionized atoms was being made on the base of technique, been developed for the alloys of replacement.

The $E_e^{(0)}$ was being defined assuming that δ – electrons were leaving the observed area and concentration of conduction electrons was staying fixed [10].

Calculating the $E_e^{(1)}$ and $E_e^{(2)}$, the model potential parameters (after quantum defect method [5]) had been taken. Fig. 5 shows the aluminum isoterms at the $0\ K\ \delta$ temperature for the different grades of ionization. So the 10% ionization results in the 15 kbar internal pressure appearance.
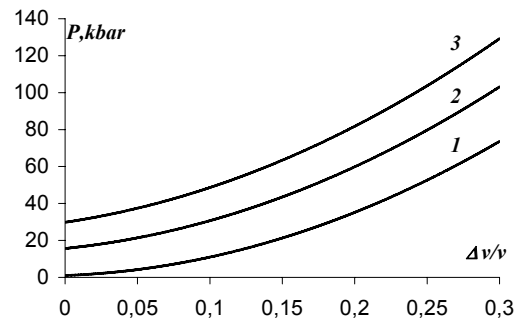

Fig. 5. Aluminum isotherms for 0 K temperature: 1 – par, 2 – 10% of ionized atoms; 3 – 20% of ionized atoms.

The consistent relations, resultant, are proposed to be engaged for studying the destruction of surfaces under the charged particles sturdy beam bombardment [6].

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