Defense Technical Information Center
Compilation Part Notice

ADP014991

TITLE: Surface Destruction and Change of Solids Properties Under the Plasma Influence

DISTRIBUTION: Approved for public release, distribution unlimited

This paper is part of the following report:

TITLE: International Conference on Phenomena in Ionized Gases [26th] Held in Greifswald, Germany on 15-20 July 2003. Proceedings, Volume 4

To order the complete compilation report, use: ADA421147

The component part is provided here to allow users access to individually authored sections of proceedings, annals, symposia, etc. However, the component should be considered within the context of the overall compilation report and not as a stand-alone technical report.

The following component part numbers comprise the compilation report:
ADP014936 thru ADP015049

Surface destruction and change of solids properties under the plasma influence.

A.L. Bondareva, G.I. Zmievskaya

Keldysh Institute of Applied Mathematics Russian Academy of Sciences

Interactions between ions beams and solids or plasma and solids result in changing of solids properties as well as ions beams or plasma characteristics. The influence of blistering on solids properties are examined in the paper. The stochastic model of blistering is presented. The evolution of distribution functions of bubbles versus bubbles sizes and coordinates in lattice is received. The depth dependences of porosity and tensions, which are created by bubbles, are calculated using the distribution functions.

1. Introduction.

The study of phenomena of interaction between plasma or ions beams and solids surface is very important for technologies. It concerns with cosmophysics, nanotechnology and controlled thermonuclear reactor. The phenomena result in change of surface relief and properties of materials. Experiments in space and thermonuclear experiments are very difficult and expensive. In this connection, computer simulation of such processes is very important.

This paper is devoted to computer simulation of fluctuation stage of high-temperature blistering. Blistering is phenomenon of development of gas bubbles in solids surface layer. Such gas bubbles are named blisters. Blistering results from irradiation of solids surface by ions of bad soluble gases. The fluctuation stage is very short, but it determines further development of blistering. The duration of the stage is 10^{-4} sec approximately. Bubbles sizes are approximately $10A$ during this stage.

The behaviour of gas-vacancy pores in Ni crystal lattice under the influence of He ions with energy from 1 keV to 35 keV and radiation dose from 10^{16} to 10^{19} ions/cm^2 is examined in this paper. Such terms can arise in solar wind and thermonuclear reactor. The temperature of material T is $0.4 \cdot T_{melt} \leq T \leq 0.6 \cdot T_{melt}$, T_{melt} is melting temperature of Ni.

2. Stochastic model of blistering and equations.

The stochastic model of fluctuation stage of high-temperature blistering had been put forward by authors [1,2]. Brownian motion model of particles with variable mass was accepted as a basis. Blistering investigation deals with computer simulation of superposition of the stochastic processes of bubbles sizes change and bubbles migration in crystalline lattice. It is possible because processes of increase of bubbles sizes and bubbles migration in lattice have appreciably different time scales. Solution of kinetic equations for Brownian motion model is non-linear problem. Therefore authors use stochastic analog method to solve these kinetic equations. Main idea of this method is change of kinetic equations by their stochastic analogs and

solution of stochastic differential equations. Scheme of splitting on physical processes and coordinates was used for solution of examined problem. The system of four stochastic differential equations was received after the splitting. Increase of size, migration on lattice, fusion of bubbles, exit of blisters on surface and bubbles destruction on it are examined in this paper. The stochastic equation for size change is following

$$\frac{dg}{dt} = -\frac{1}{kT}D(g,t)\frac{\partial \Delta\Phi(g,\vec{r},t)}{\partial g} - \frac{1}{2}\frac{\partial D(g,t)}{\partial g} + \sqrt{2D(g,t)}W_g(t)$$

$$t_0 \leq t \leq T_k, \quad g(t_0) = g_0 \in [g_{0min}; g_{0max}], \quad g(t) > 2$$

g is bubble size, $\Delta\Phi(g,\vec{r},t)$ is Gibbs potential, $D(g,t)$ is diffusion coefficient in sizes space, $W_g(t)$ is Wiener process, T_k is duration of fluctuation stage. $\frac{\partial \Delta\Phi(g,\vec{r},t)}{\partial g}|_{g=g_{cr}} = 0$, g_{cr} is "critical" size of blister.

$$\Delta\Phi(g_{0min},\vec{r},t) = \Delta\Phi(g_{0max},\vec{r},t) = \Delta\Phi(g_{cr},\vec{r},t) - kT,$$

$$g_{0min} < g_{cr} < g_{0max}.$$

$\Delta\Phi(g,\vec{r},t)$ and $D(g,t)$ nonlinearly depend from bubble size. Heterogenous condensation on bubbles surfaces, difference between chemical potential of phases, surface tension on bubbles surface, elastic reaction of solids lattice, nonequivalence of bubbles position in lattice, break of connections of crystal lattice are considered using $\Delta\Phi(g,\vec{r},t)$ and $D(g,t)$.

The stochastic equation for depth is following

$$z(t) = z(t_0) + \int_{t_0}^{t} H_z(\tau,x(\tau),y(\tau),z(\tau))d\tau + + \int_{t_0}^{t} \sigma(\tau,z(\tau))dW_z(\tau)$$

$$H_z(\tau,x(\tau),y(\tau),z(\tau)) = -\frac{1}{\gamma M_g}\frac{\partial U}{\partial z} - \frac{1}{2}\frac{\partial D_z}{\partial z}$$

$$\sigma_z(z,t) = \sqrt{2D_z(z,t)} \quad U = U_{bb} + U_{bs}$$

W_z is Wiener process, z is depth of bubble from surface under irradiation, M_g is blister mass, x,y,z are bubble coordinate in crystal lattice, D_z is diffusion coefficient, U_{bb} is interaction potential between blisters by phonons and oscillation of electron density, U_{bs} is potential of

interaction between bubbles and surface.

$$U_{bb} = \sum_{j \neq i}^{N} [\frac{0.6 \cdot b_r + a_r \cos(c_r(\vec{r}_i - \vec{r}_j))}{|\vec{r}_i - \vec{r}_j|^3} -$$

$$b_r \frac{(x_i - x_j)^4 + (y_i - y_j)^4 + (z_i - z_j)^4}{|\vec{r}_i - \vec{r}_j|^7}]$$

a_r, b_r c_r are model coefficients, $\vec{r}_i$ and $\vec{r}_j$ are radius-vector of two interactive bubbles. Two bubbles can fusion if fusion condition is carried out. The fusion condition is $|\vec{r}_i - \vec{r}_j| \leq \frac{r_{He}}{a}(g_i^{1/3} + g_j^{1/3}) + \Delta_f$. Δ_f is model parameter. $0 \leq \Delta_f \leq a$, a is lattice parameter, r_{He} is radius of He atom.

Authors modified Artem'ev method to solve the stochastic equations and used new method to solve system of four concerned with each other stochastic equations with nonlinear coefficients.

The developed model allows to receiv the following characteristics: distribution function of bubbles from bubbles size and position on crystal lattice, mathematical expectations and dispersions of bubble size and distance from surface, evaluations of porosity of solids layers and tensions in layers.

3. Conclusions.

1. According to classical theory bubbles destroy if their sizes are less than g_{cr} and bubbles increase if their sizes are more than g_{cr}. However, numerical experiments demonstrate that blisters can increase if their sizes are more than g_{0min} and less than g_{cr}. Bubbles can destroy if their sizes belong to interval from g_{cr} to g_{0max}. The part of increased blisters with sizes $\in [g_{0min}; g_{cr}]$ is larger than the part of destroyed blister with sizes $\in [g_{cr}; g_{0max}]$.

2. The bubbles migration into the surface under irradiation if bubble radius is less than 5 A, otherwise bubbles stop;

3. Layer-like structure of near-surface layer is discovered. Layers with accumulation of bubbles alternate with layers where number of blisters is small;

4. The greatest porosity is observed on depths of $\sim 0.85 \cdot R_p$ and $\sim 0.35 \cdot R_p$, R_p is middle depth of projection run; The porosity of solid layers from depth at time of finish of fluctuation stage is shown on Figure 1. The depths of two biggest maximums of porosity correspond to depths of development of two kinds of blisters. The depth $\sim 0.85 \cdot R_p$ conforms to depth of "large" bubbles. And the depth $\sim 0.35 \cdot R_p$ agrees with "small" bubbles.

5. Rate of increasing of bubble size reduces if blister size is bigger than 12 A. This phenomenon connects with great number of connections breaks in crystal lattice;
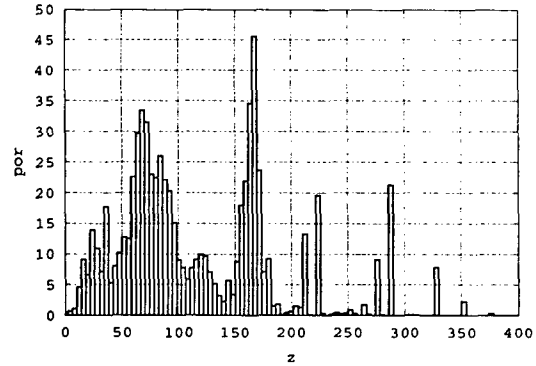

Figure 1: The porosity of solid layers from depth at time of finish of fluctuation stage is represented on this picture. The depth from surface (z) is measured in lattice parameters. 0 is surface. 400 corresponds to $2 \cdot R_p$. The porosity is considered as ratio of layer porosity from porosity of all sample at initial time.
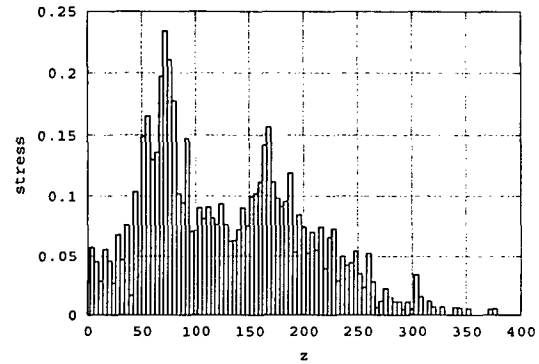

Figure 2: This figure shows the tensions in solid layers at finish time. The tension is measured in $2 \cdot 10^9 Pa$. The depth from surface (z) is measured in lattice parameters. 0 is surface. 400 corresponds to $2 \cdot R_p$.

6. Tensions in solid layers at finish time are shown on Figure 2. Largest tensions are observed on depths $\sim 0.85 \cdot R_p$ and $\sim 0.35 \cdot R_p$. Stress is pronounced near surface.

7. Distribution functions of bubbles from sizes and coordinates in lattice are nonequilibrium.

4. References

[1] A.L. Bondareva, G.I. Zmievskaya, *in book Mathematical Models of Non-Linear Excitations, Transfer, Dynamics and Control in Condensed Systems and Other Media*, Plenum Publishing Corporation, editor L. Uvarova, New-York (1998) 241.

[2] A.L. Bondareva, G.I. Zmievskaya, *XXV ICPIG Proceedings* 3 (2001) 187.