THE SYSTEM “CO_2 LASER + ION SOURCE” AS A STIMULATOR TO NONADDITIVE PROCESSES ON A METAL SURFACE

S.P. Bakanov and B.N. Poizner

Tomsk State University
Received July 26, 1995

A hypothesis that joint action (coaction) in a system “solid body–plasma–energy flows (flows of matter)” is nonadditive, as well as some new synergistic peculiarities of system evolution, is discussed. A scheme of a priori combination of actions is also considered. The structure of a program package for investigation of the evolution of target matter under coaction of concentrated energy flows (CEF's) of various types is analyzed. The prospects for computer-aided creation of physical and mathematical models starting from chosen conditions are also under discussion. A model is presented of metal thermal oxidation by an oxygen-ion beam upon exposure to laser radiation, as well as a model of laser-arc melting of metals and preliminary results of simulation.

It seems expedient to consider the role of the pulsed lasers in the context of creation of new technologies based conceptually on the nonlinear physics ideas harnessing the action of concentrated energy fluxes (CEF's) of different nature on matter. Among promising ways for action, beams of charged particles (ions, electrons, and so on), fields nonuniform in space and time, and so on, should be pointed out. Clearly, the CEF different nature is tentative, and we can say about it only for macrodescription of processes.

For the theoretical description, synergism of processes occurring in the matter irradiated by CEF is of interest. As an example, Refs. 2 and 3 should be mentioned. We have to certify lack of theoretical investigations of joint action (coaction) of several CEF's of different nature.

Coaction occurs when CEF's:

– affect a set of general parameters of a medium;

– engender, support, and control the same or correlating processes (heat transfer, phase changes, diffusion, macrokinetic processes, and so on);

– coexist in time and act on common or contiguous space.

The hypothesis that coaction is nonadditive seems justified, i.e., some new synergistic peculiarities in evolution of investigated systems appear under coaction of two and more CEF's of different nature.

We restrict ourselves to the consideration of only a solid body (SB) and a space surrounding it as an object of action. Therewith, interaction of subsystems in the given system would be expected like that shown in Fig. 1*a*.

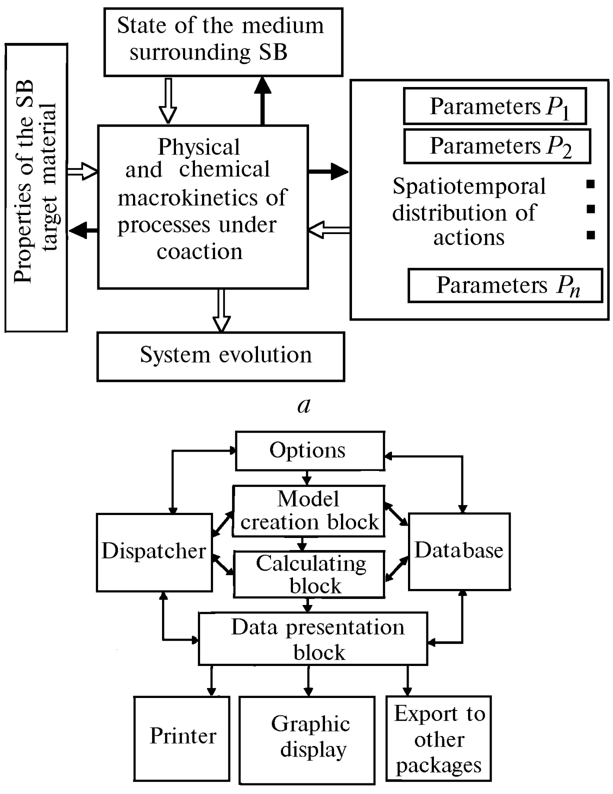


FIG. 1. The structure presentation of factors determining the system evolution. Here P_1, P_2, ..., P_n are the concentrated energy fluxes of different nature (a). The flow chart of the program package for simulation of coaction on different solid bodies (b).

0235-6880/96/02 154-04 $02.00

We suggest the universal instrument for theoretical study of the evolution for a variety of states of target matter upon exposure to the CEF of all types: from mechanical pressure to X-ray irradiation. It consists of the computer-aided simulation of physical and mathematical models by stages (with conditions chosen by a researcher: object of coaction, characteristics of coaction, state of a medium surrounding a target, model approximation, and so on), their subsequent comprehensive study and refinement, and comparison with the use of the general-purpose program package. The package structure is shown in Fig. 1*b*. In this case, the objective is the development of physical basis for the technology capable of realizing principally new mechanisms of self-organization of the internal structure of materials with the help of multiplicative effect of all actions and control over nonequilibrium state of processes in a set of coupled subsystems.

By the present time, some fragments of the package considered above have been realized: some calculating modules (integration of systems of differential equations by the modified Runge-Kutta-Merson method and check of solution stability by the Routh-Hurwitz method), interface elements, and database. This allows one to study the system evolution in some concrete cases.[4-6] As an illustration, we consider briefly two models: (1) point-process model of the thermal oxidation of metal like wolfram with metallic oxide being sublimated easily upon exposure to an ion beam in the laser radiation field[4] of a pulsed CO_2 laser and (2) the model of processes under coaction of electric arc and laser radiation on a metal.[5]

1. Temporal evolution of the system "solid body (metal+oxide on its surface) − plasma cloud (for the most part, WO_3 ions) − laser beam − oxide ion beam" can be described by dynamics of four variables, with X and Y being the amount of oxide on the metal surface and within the cloud, respectively, T and $\mathcal{T}$ being the average temperature of the S" and cloud, respectively.

The model is described by self-consistent system of the ordinary nonlinear differential equations

$$\frac{dX}{dt}=\frac{\alpha_1}{X}e^{-\alpha_2/T}+\alpha_3-\alpha_4\,e^{-\alpha_5/T}-\frac{\alpha_6}{X}[1-\exp(\alpha_7\,Y-\alpha_8)],$$

$$\frac{dY}{dt}=\alpha_9\,e^{-\alpha_5/T}+\frac{\alpha_{10}}{X}[1-\exp(\alpha_7\,Y-\alpha_8)]-\alpha_{11}\frac{Y}{\mathcal{T}}-\alpha_{12},$$

$$\frac{dT}{dt}=\alpha_{13}\,X^2\exp\left[\frac{-\alpha_{30}\,Y^2}{(1-Y)^{1/2}\,\mathcal{T}^{3/2}}\right]+$$
$$+\alpha_{14}\exp\left[\frac{-\alpha_{30}\,Y^2}{(1-Y)^{1/2}\,\mathcal{T}^{3/2}}\right]+\alpha_{15}-\tag{1}$$
$$-\alpha_{16}Y+\frac{\alpha_{17}}{X}\,e^{-\alpha_2/T}-\alpha_{18}\,e^{-\alpha_5/T}-(\alpha_{19}\,T-\alpha_{20}\,\mathcal{T})-$$
$$-(\alpha_{21}\,T^4-\alpha_{22}\,\mathcal{T}^4),$$

$$\frac{d\mathcal{T}}{dt}=\alpha_{23}-\alpha_{23}\exp\left[\frac{-\alpha_{30}\,Y^2}{(1-Y)^{1/2}\,\mathcal{T}^{3/2}}\right]+\alpha_{24}Y+$$
$$+(\alpha_{25}\,T-\alpha_{19}\,\mathcal{T})+(\alpha_{26}\,T^4-\alpha_{27}\,\mathcal{T}^4)-\alpha_{28}\,\mathcal{T}+\alpha_{28}\,\alpha_{29},$$

where $\alpha_1-\alpha_{30}$ are the dimensionless coefficients independent (for the given model) of X, Y, T, and $\mathcal{T}$. The first and third equations of the system describe the thermal balance for the S" and cloud matter, respectively; the second and fourth equations describe the exchange with matter between the S", cloud, and environment.

In Fig. 2*a*, factors and near-surface processes are shown considered in the derivation of Eq. (1). The order of terms in the right-hand side of both systems is the same.

Equations for these processes were derived on the basis of the model from Ref. 2. The following basic approximations were used (see Fig. 2*b*):

− the target was considered uniform with a flat surface, thermally thin, in a vacuum;

− back and side walls of the S" were thermal insulated;

− flows covered the surface uniformly and were incident perpendicular to it;

− laser and ion beams were continuous, stationary, and nonmodulated; $E_{\text{ion beam}}\in[0.5;\,5]$ keV; the charge of the ion beam was compensated by the ion background, and laser radiation was emitted in the IR range;

− $T\in[20;\,3420[$ °C;

− only reaction of the type $2W + 3O_2 \rightarrow 2WO_3$ ran in the system, the oxide film was formed by WO_3, it was thin, uniform, plane, and parallel to the target surface;

− Y was the average amount of matter in the cloud, $\mathcal{T}$ was the average cloud temperature, V_{cloud} = const, and $\sum_i q_i = 0$;

− only surface processes were considered in the S";

− the matter condensed within the cloud did not come back to the surface; condensation on the S" was neglected;

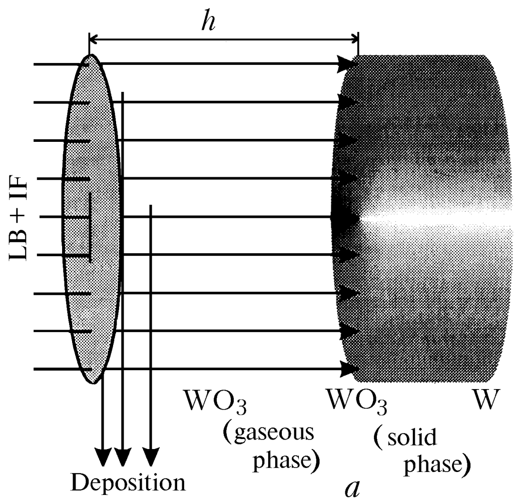
− the sublimation process was independent of the incident flow;

− the model of point process was considered;

− flows did not interact with each other and did not scatter.

A run of computer experiments was performed. Their results allowed us to make the following conclusions:

− behavior of nonstationary processes depends on the intensity of each beam; the process develops into oscillatory one with the intensity exceeding some threshold values of the beams intensities, i.e., the Hopf bifurcation is observed (Figs. 3 *a* and *b*); this agrees with the experimental data obtained elsewhere[7];



a

$$\frac{dX}{dt} = \boxed{\text{oxidation on the SB surface (by Vagner)}} + \boxed{\text{nonequilibrium addition}} - \boxed{\text{sublimation from surface}} - \boxed{\text{surface pickle}} + \dots ,$$

$$\frac{dY}{dt} = \boxed{\text{sublimation from surface}} + \boxed{\text{surface pickle}} - \boxed{\text{condensation}} - \boxed{\text{forced clearing off}} + \dots ,$$

$$\frac{dT}{dt} = \boxed{\text{laser beam energy incident on the SB}} + \boxed{\text{ion beam energy incident on the SB}} + \boxed{\text{energy evolved at oxidation}} - \boxed{\text{energy absorbed at sublimation}} \mp \boxed{\text{heat exchange between cloud and SB}} + \dots ,$$

$$\frac{d\mathscr{M}}{dt} = \boxed{\text{laser beam energy contained in cloud}} + \boxed{\text{ion beam energy contained in cloud}} \pm \boxed{\text{thermal exchange between cloud and SB}} - \boxed{\text{energy transfered to refregirator}} + \dots .$$

b

FIG. 2. Physical model of the W-type metal thermal oxidation (a) (see the system of eqXations (1)) and the simplest model of coaction (b) (see the text and Ref. 4).

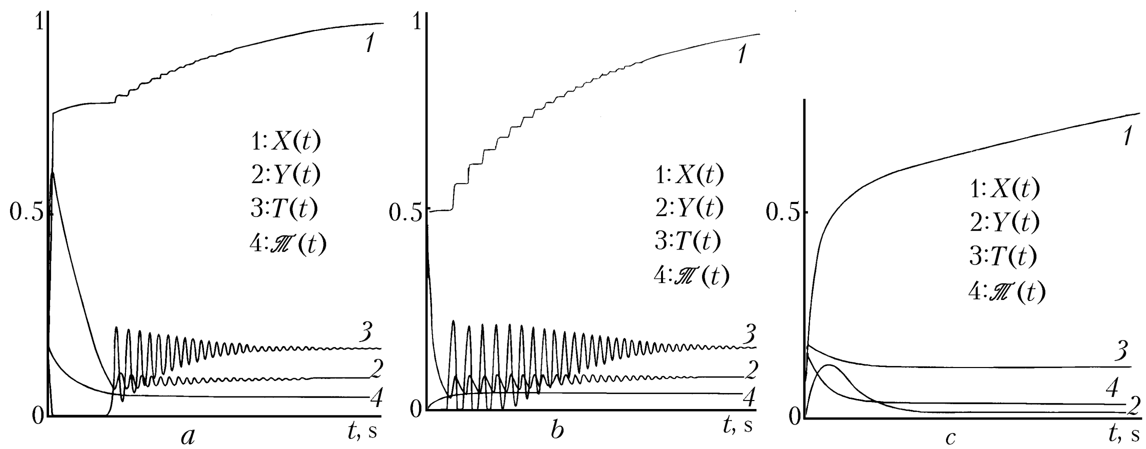


FIG. 3. ResXlts of compXter-aided simXlation of oxidation of the W- type metal Xpon exposXre to a laser beam (see Ref. 4 and Eqs. (1)): (a) test problem (with parameters close to that observed in the experiments performed by Xs in Ref. 2); (b) example of the system temporal evolXtion with the initial conditions being changed, i.e., the stationary conditions are the same as for the test problem (see Fig. 3 a); (c) example of beams with prethreshold intensities I_{LB} = 21000 and I_{IB} = 50000. Oscillatory state is not established.

– dependence of the system evolution on the initial values of variables has not been found (Figs. 3 *a* and *b*); this does not contradict Ref. 3;

– the process character somehow depends on the intensity of heat exchange between subsystems "solid body – cloud" and "cloud – refrigerator"; this is explained by physical conditions, for instance, the system may transform itself into strange attractor for appropriate combination of its thermal characteristics;

– the model and corresponding program module are efficient within a relatively wide range of variation of the parameters of the given problem and similar ones.

2. We consider further the processes of the plasma density and temperature variations under the coaction of the laser radiation and the electric arc on the target melting pool. Initial are the point-process models of molecules' dynamics and temperature of an erosion flare for resonant absorption of laser radiation acting on the metal.[6,7] The model is characterized by the following factors:

– increase of the plasma density due to photoionization processes caused by the high intensity of laser radiation and high electron energy is considered;

– dynamics of the vapor concentration is described more accurately than in Refs. 6 and 7;

– thermal losses due to plasma emission and temperature drop caused by interaction between the electron and ion plasma components are considered;

– the "saturated" vapor concentration is reduced to the initial conditions;

– the extent of a plasma flare along the laser beam is taken into account relative to the distance between the anode and cathode of an electric arc tube;

– screening of laser radiation by plasma is described.

The following approximations were used:

– point–process model;

– the model was taken beyond the scope of the Stefan problem because of the absence of temporal dependence of phase boundaries;

– only two degrees of freedom of plasma were considered, what narrows down the possibilities to explain some collective phenomena;

– some peculiarities of the mechanisms of plasma energy absorption in metal were neglected.

Results of computer experiment based on the given model for special cases considered here agree with the conclusions of Refs. 3, 6, and 7. In particular, a possibility of phase correlation for oscillations of plasma concentration observed during simulation in the cloud with periodical variations of the laser beam intensity is confirmed by the method of improving the characteristics of annealing described in Ref. 8.

"oth models considered here claim only to qualitative description of corresponding system evolution. This is primarily due to uncertainty of many physical constants in equations and with lack of possibility to perform field experiments now. Nevertheless, results obtained do not reject the initial hypothesis that coaction is nonadditive and provide a basis for creation of metamodel of complex manifestation of open nonequilibrium systems.

Further steps on this way, in our opinion, should be following:

– performing a series of field experiments with the aim of successive refinement of the above-mentioned models of nonequilibrium processes and their subsequent use for verification of the system for creating computer models of nonequilibrium processes under coaction of different nature;

– determination of conditions of dynamic chaos and bifurcation by way of new computer experiments;

– comparison of temporal evolution of a system under joint action of two flows of different nature and of the same nature (for example, oxidation of W in the oxygen atmosphere upon laser irradiation[3]);

– conversion to extended models.

ACKNOWLEDGMENT

We would like to acknowledge E.V. Kartaev for useful discussions and kindly presented results.

REFERENCES

1. G.A. Mesyats, V.V. Osipov, and V.F. Tarasenko, *Pulsed Gas Lasers* (Nauka, Moscow, 1991), 200 pp.
2. F.V. Bunkin, et al., Izv. Akad. Nauk SSSR, Ser. Fizika **45**, No. 6, 1018–1042 (1981).
3. T.S. Achromeeva, et al., *Nonstationary Structures and Diffusion Chaos* (Nauka, Moscow, 1992), 544 pp.
4. S.P. Bakanov, D.V. Saf'yanov, and B.N. Poizner, in: *Abstracts of Reports at the 8th International Conference on Radiative Physics and Chemistry of Inorganic Materials,* Tomsk (1993), Vol. 1, p. 47.
5. S.P. Bakanov and E.V. Kartaev, in: *Abstracts of Reports at the 4th Russian Scientific Students' Conference,* Tomsk (1994), p.30.
6. S.P. Bakanov, D.V. Saf'yanov, and B.N. Poizner, in: *Abstracts of Reports at the 8th International Conference on Radiative Physics and Chemistry of Inorganic Materials,* Tomsk (1993), Vol. 1, p. 82.
7. A.A. Mal'gota, Kh.M. Bakhir, and A.A. Shiyan, Fizika i Khimiya Obrabotki Materialov, No. 3, 86–97 (1991).
8. M.A. Cross, U.S. Patent No. 500688 (April 9, 1991).