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Patterning and pattern selection in a surface layer: Feedback between point defects population and surface layer temperature variations

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HIGHLIGHTS

- Particle irradiation of thin foils leads to point defects patterning on a surface layer.
- A local temperature is larger in vacancy enriched domains comparing to that in a bulk.
- A coupled dynamics of layer temperature and defect concentration leads to pattern selection.
- Defect production rate affects a morphology of vacancy enriched domains.

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ABSTRACT

We study dynamics of pattern formation in a prototype system of nonequilibrium point defects in thin foils under sustained nonequilibrium conditions. A reaction–diffusion model describing spatio-temporal behaviour of both vacancy population and local temperature of a surface layer is used. It is shown that pattern selection processes caused by coupling between defect population and local temperature of a surface are realized. Associated oscillatory dynamics of main statistical moments of both vacancy concentration field and surface layer temperature is analysed in detail. It is found that during the system evolution spatial distribution of local temperature variations of the surface layer relates to vacancy population distribution. It is shown that the mean size of vacancy clusters (from 30 nm up to 300 nm) evolves in oscillatory manner due to pattern selection processes. Morphology of defect complexes can be controlled by defects generation rate.

1. Introduction

It is well known that self-organization of defect structure accompanied by nano-structures formation on solid surfaces is a result of rearrangement of mobile point defects produced by nonequilibrium conditions. Such defects are generated due to structural disorder production caused by sample heating, at laser pulse irradiation or at displacement of atoms in cascades at particle irradiation. Defects are able to move along the sample and to the surface, and arrange in complexes due to spatial instabilities resulting in formation of surface structures like dots having sizes of nano- or micrometres in surface layer of semiconductors or metals; formation of stacking faults in a bulk [1]. It is well known that depending on irradiation conditions (defect production rate and temperature) point defects can arrange into objects of higher dimension such as

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clusters (di-, tri-, tetra-vacancy clusters), defect walls with vacancy and interstitial loops [2,3], voids [4], precipitates [5] and bubble lattices [6–8]. Nano-structured thin films fabricated in this way can be used to study mechanisms of defects clustering, microstructure change at applied nonequilibrium conditions, from the one hand, and, from the other one they can be exploited for developing novel electronic devices, memory storage, detectors, etc.

In general, a production of defects in crystals under both equilibrium (by heating the system) and nonequilibrium (laser or particle irradiation, mechanical loadings) conditions leads to an emergence of uncompensated strains and local deformation of the lattice. These deformations can be compensated by rearrangement of defects due to their interaction with inhomogeneous deformation field. This results in a formation of small clusters of point defects (stacking faults). In such a case a formation of clusters of defects is governed by deformation-induced or strain-driven instabilities [9]. Moreover, local temperature variations can lead to a change in both mobility of defects and rate of their recombination. The local temperature may differ from that of the bulk even in equilibrium conditions. It leads to an emergence of thermal gradient responsible for the Soret-like diffusion of mobile species (defects) and their agglomeration (see, for example, Refs. [10,11]). Once the temperature distributed over local defects attains its bulk counterpart, the system gets equilibrated and pattern-like structures appear. By considering crystalline systems under nonequilibrium conditions, one should take into account that point defects are produced constantly. Defects produced by laser or particle irradiation have enough energy to migrate along the crystal to compensate local lattice deformation due to pairwise defect–defect interaction [12]. Moreover, a production of defects under nonequilibrium conditions can lead to a supersaturation of defects with accumulated elastic energy in point defect spots resulting in certain pattern-like accumulations and formation of cavities. Therefore, pattern formation of accumulated defects occurs inevitably.

To consider point defects self-organization under nonequilibrium conditions, usually, one uses a theory of quasi-chemical reactions, where concentrations of point defects play a role of dynamical variables. Quasi-chemical reactions correspond to defects production, their annihilation, formation of complexes, etc. The corresponding diffusion fluxes should be taken into account due to point defects are mobile species. Generally, the related dynamical models incorporate the defects ensemble environment changes (emergence of uncompensated stresses caused by defects formation, local temperature variations in processes of defects formation, their interactions and rearrangement). One of the interesting problem related to above processes lies in a determination of distribution of elastic and temperature fields conjugated to point defect concentration. An emergence of mechanical stresses in the surface layer caused by a production of mobile nonequilibrium point defects in foils leads to mechanical stresses in the surface layer. This results in self-organization of nano-structures leading to compensation of such stresses. In Refs. [13–15] it was shown that dynamics of point defect concentration interacting with a deformation of the stretched surface layer can be described by nonlinear equation of reaction–diffusion kind. This model does not adopt a surface height change directly, as far as no sputtering and erosion of the surface is assumed. In such a case one deals with point defects rearrangement in surface layer of the foil, not sputtering effects (see Ref. [16] and citations therein). As far as all above fields are coupled, therefore, during the system evolution self-organization processes can be seen through spatio-temporal instabilities leading to pattern formation, oscillatory dynamics of main variables, change in geometrical characteristics of point defects patterns. Inhomogeneity of point defects spatial distribution should be accompanied by inhomogeneous distribution of temperature and elastic fields. Therefore, generally, one should expect temperature field patterning at formation of defect structures. Temperature patterning in a surface layer was discussed previously for adsorptive layer systems, where local surface layer temperature varied according to rearrangement of atoms adsorbed from gaseous phase (see Ref. [17]). The similar effects were discussed in a class of systems manifesting epitaxial growth with pyramidal structures formation on a surface (see Ref. [18]). This spatio-temporal problem remains actual during the last decade in nonlinear systems, whose dynamics and diffusion processes strongly depend on temperature fluctuations (nano-systems, systems with nano-metre objects). Its solution allows one to study in detail physical mechanisms of mobile species patterning and consider pattern selection processes, not discussed previously for such a class of systems. The main idea and novelty of this work lie in a solution of this problem.

Usually, considering dynamics of defects one admits that the temperature of the irradiated sample remains constant due to high thermal conductivity (for example, for metals). This effect is possible for massive samples and realized in a bulk of the material. Considering thin films/foils (with thickness $\sim$0.5 μm) as a sample in an environment characterized by a constant temperature T_0 one deals with processes of local changes in the sample temperature T due to heating, production of defects and their annihilation (a range of ionizing particles is smaller than thickness of the sample). A local increase in the sample temperature results in defects annealing. It leads to defect energy release into a heat increasing the temperature of the sample. As a result a number of defects decrease with increasing the heat transfer. Next, the sample cools, heat transfer decreases and new defects accumulate. A repetition of this scenario leads to self-oscillations of the sample temperature and point defects concentration. An emergence of such self-oscillations in homogeneous systems was reported in Refs. [19,20]. There are many experimental observations of self-organization of point defects in solids with spatio-temporal oscillations of point defect concentration (see, for example, Refs. [21–23]). Among them one can note: void size oscillations were observed in irradiated nickel samples [24]; temperature oscillations of crystals CH_4 were reported in Ref. [22]; periodic variations of microhardness of Nimonic 90 with γ-precipitates with radiation dose growth were discussed in Ref. [25]; periodic variation of electric resistivity of irradiated copper and aluminium was shown in Refs. [26–28].

In this work we study spatio-temporal evolution in a prototype model of the nonequilibrium system of point defects following the approach developed in Refs. [13–15], where local temperature field in surface layer evolves according to main mechanisms discussed above [19,20]. We consider metallic foils under particle irradiation as an object of our study by taking