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COMPUTER SIMULATION OF THERMAL CYCLING OF POROUS COATINGS: HYBRID EXCITABLE CELLULAR AUTOMATA METHOD

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Thermal barrier coatings (TBC) are currently widely used to improve the heat resistance of critical parts, in particular cooled blades of gas turbine engines [1]. The thermal barrier coating deposited on the top of a high-temperature alloy substrate is typically a sandwich-like structure consisting of the i) metal substrate, ii) metallic bond coating, and iii) an outer ceramic layer with low thermal conductivity. A real solid is a hierarchically organized system that contains a set of interfaces, or independent 2D subsystems, where rotational wave-, mass- and energy fluxes occur [2-5]. The rotational-wave fluxes are particularly intensify under dynamic loading conditions in wide range of applications – for example, in friction [3] or in plasma environment [6,7]. The rotational modes of deformation arise due to the action of the local moments of forces. In the stochastic excitable cellular automata (SECA) method, the simulated specimen is represented as a cellular automaton, i.e., a set of ordered active elements each of which imitates a part of the material contained in a certain volume of space. In doing so, it is characterized by the following numerical parameters: heat capacity and thermal conductivity. The network of the cellular automaton elements is divided into "clusters", whereas each one models a separate grain with its own crystalline lattice orientation characterized by the Euler angles ψ, φ, η Note, that the proposed algorithms for thermal and mechanical energy transfer within the grains are isotropic, i.e. directionally independent. This, in fact, limits the model. Thus, the anisotropy of the grain structure arises only at the grain boundary regions through the angle of misorientation with the neighboring grain. The details on new realization of the Excitable Cellular Automata approach might be found elsewhere [2,4,8].

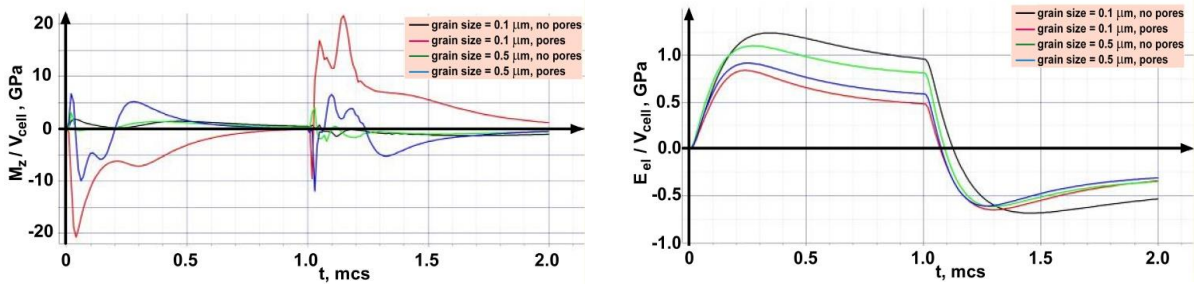
A series of numerical experiments on cyclic thermal loading of three-layered composites with intermediate layers possessing different structures was carried out by the SECA method. Each specimen measured 5×2×5 μm^3, the diameter of the active element was 0.1 μm. The loading scheme and the general view of the specimens are shown in Fig. 1.

(a) (b)

Fig. 1. Loading scheme of specimens (a), general view of a specimen (b)

The numerical simulations yielded the time dependences of the mass-averaged values of the moment of force and "effective" stress as plotted in Fig. 2. As is seen from the curve shown, the maximum values of the moment of force are achieved for the specimen with the intermediate nanoporous sublayer with grain size of 0.1 μm. This suggests that a large part of the energy of internal thermal stresses is expended for the formation of microvortices. The latter results in elastic energy dissipation and its transfer to the entropy component of the total accumulated energy. This conclusion

is confirmed by the analysis of the diagram in Fig. 2b. It shows the time dependences of the average thermal stress within the intermediate sublayer at variation of the microstructure parameters.



(a) (b)

Fig. 2. Time dependences of the specific moment of force (a) and effective stress (b) averaged over the component mass in the studied compositions. Black graph – grain size = 100 nm and no pores, green – grain size = 500 nm and no pores, red – grain size = 100 nm and pore size = 100 nm, blue – grain size = 500 nm and pore size = 500 nm

It was found that thermal cycling of a polycrystalline system is responsible for arising high microstresses coming from the thermal expansion anisotropy of grains. In this regard, along with accounting for the local rotational modes of structural elements and thermal radiation from the pore walls, it is important to account for the material's ability to reversible structural transformations in the pore walls. The reversible structural transformations would accumulate peak energy values in elastic rotational stress fields, which are of inertial nature, to prevent the formation of thermal fatigue cracks. The stress level was shown to decrease with increasing fraction of rotational modes. This tendency was observed over the entire depth of the studied specimen and during the entire thermal loading time. An optimal porosity value for the intermediate sublayer was determined at which the structure exhibits the best relaxation capacity. Thus, the introduction of certain porosity in the intermediate sublayer can exert a positive effect on the service life of the thermal barrier coating.

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