The influence of glass surface multifractality in glass nucleation.

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In this paper we present a numerical model that incorporate the algorithm to simulate surface nucleation in circumstances of surface multifractality. Surface roughness is caracterized by Holder exponent and this model includes it in rate nucleation expression. The simulations is made in both one dimensional and bidimensional surface profiles.

Introduction

Nucleation and crystallization of glasses continue to attract fundamental and technological interest.Mechanical damage is known to promote surface nucleation of glass [1-4] but the nucleation mechanism is not well understood.It is confirmed [5-8] for cordierite, diopside lithia-alumina-silica and float glasses that sharp edges or tips are favoured nucleation sites.AFM experiments for industrial glasses like float glass demonstrate the self-affinity of glass surface [9]. Also, AFM experiments have been performed on fractured surfaces [10-11] of soda-lime glass resulting from fracture. It leads to the finding that fractured surface is multifractal (multi-affine).The first model of influence of surface roughnees on crystallization of glasses is proposed by Smeltzer et.al [12].

Model

For a self-affine function h(x) we have $h(x) = b^{-H} f(bx)$ where H is called the Holder exponent and give a quantitative measurement of the "roughness" of the function h(x).More generally, let us denote M(q, l) the order q of absolute moment of $\delta_l h(x) = h(x+l)-h(x)$:$M(q,l)=<|\delta_l h(x)|^q>$ where < > mean mathematical expectation .

If $M(q,l)\sim C_q l^{Hq}$ where C_q is a prefactor and H_q is a nonlinear function of q the function h(x) is multifractal. In our model function h(x) represent surface profile discretized in N points, $h(x_i)$, i=1…N. The simulations are made under isothermal conditions. We consider the fact that surface roughness reduce energy barrier to nucleation in a simple manner: the probability of nucleation in the point x_i is $P_i = Ce^{\frac{-E+C\cdot H_i}{T}}$ where H_i is local Holder exponent and C is a prefactor.

In simulation desorbtion phenomena are prohibited.

The steps of the algorithm are:

1. A surface profile weight with prescribed Holder exponent is generated $H(x_i)$;

for count = 1 to maxiterations.

2. Compute for each point x_i(i=1…N) the probability of nucleation in $P_i = Ce^{\frac{-E+C_y \cdot H_i}{T}}$

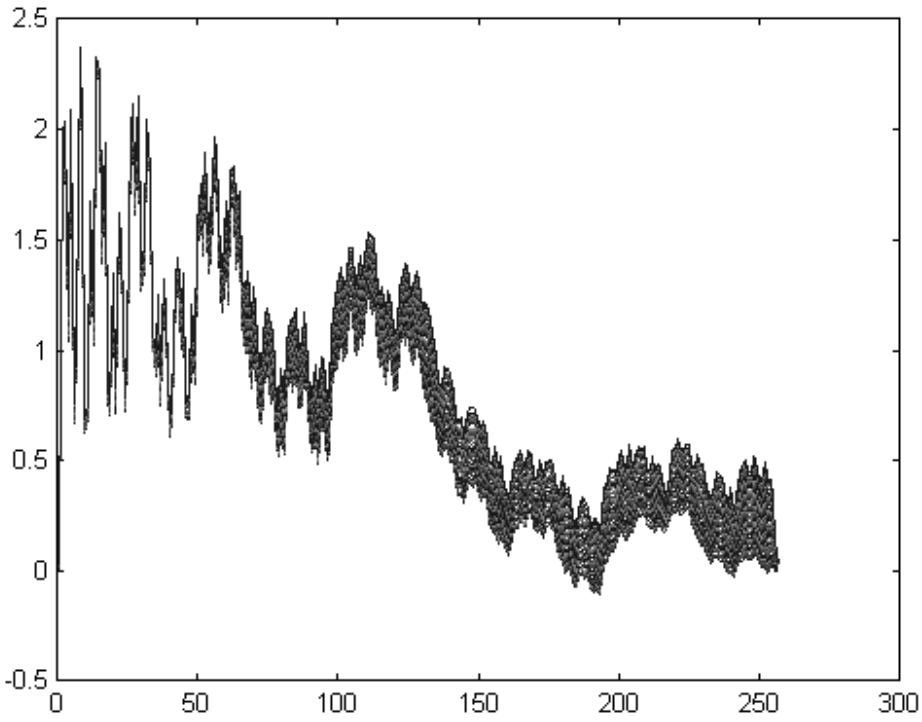
3. Generate a random number γ_i, $\gamma \in [0,1]$.

4. If $P_i \geq \gamma_i$ then in point x_i the surface profile $H(x_i)$ is increased by a small quantity δ.

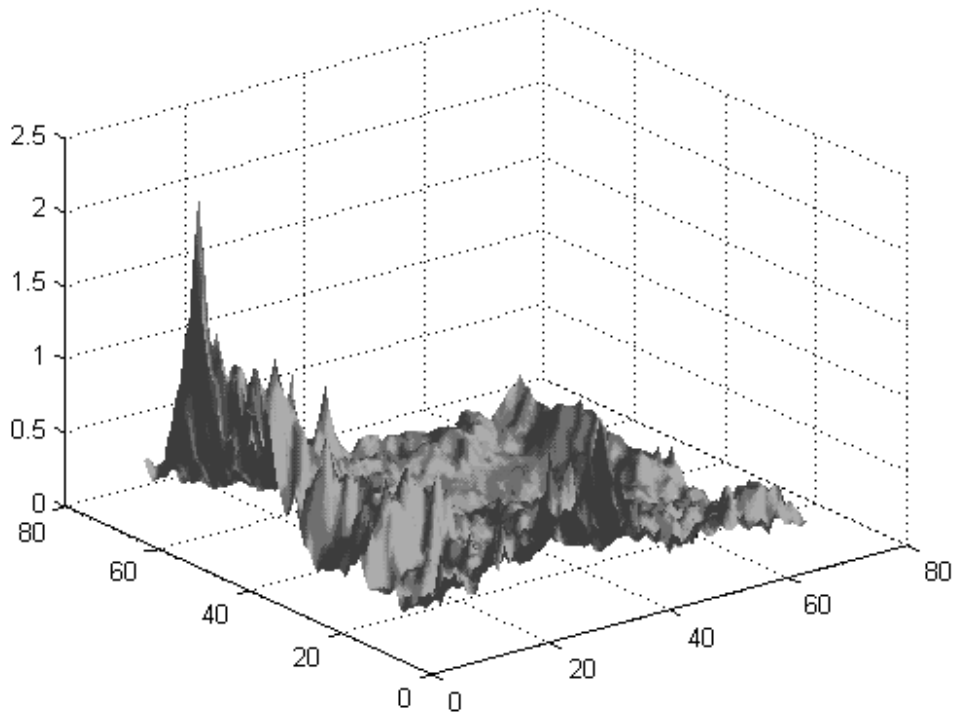
end

Results and conclusions

In the next two figures we present the results of the simulations. The nucleation sites appear to be in concordance with basic assumption of the model that mean the fact that the probability expression was well chosen. The important remark is the fact that multifractal character of surface is preserved during simulated nucleation process.



One-dimensional simulation. The initial surface profile have a prescribed Holder exponent H(x)=abs(x^0.5)



Two-dimensional simulation. The initial surface profile have Holder exponent H=0.5. The only difference between initial and final surface is shown

As concluding remark, we note that the basis of the model presented in this paper is quite general: it should be possible to incorporate additional nucleation scenarios into the model by appropriately modifying the probability function.

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[1] G.Partridge, P.W. Mc.Millan, Glass Technol. 15 (1974) 127

[2] G. Partridge, Glass Technol. 28 (1987) 9

[3] Y.Ding, A.Osaka, Y.Miura, J.A.Ceram.Soc. 77 (1994) 749

[4] G.Morgensen, N.H.Christensen, Phys. Chem. Glasses 22 (1981) 17

[5] R.Muller, S.Reinsch, G.Volksck, K.Heide, Ber. Bunsenges, Phys. Chem. 100 (1996), 1438

[6] R.Muller, S.Reinsch, W.Pannhorst, Proceedings of the 11th Conference on Glass and Ceramics, Varna 1993, 63-68

[7] J.Schmelzer, J.Moller, I.Gutzow, R.Pascova, R.Muller, W.Pannhorst, J.Non. Cryst. Solids 183 (1995) 215

[8] S.Reinsch, R.Muller, W.Pannhorst, Glastech. Ber. Glass Sci. Technol. 67C (1994) 432

[9] D.Abrion, Y.Levillain, H.Arribast, F.Creuzet, Proceedings of the International Symposium on Glass Problems, Istanbul, 1996, p.427

[10] B.Nghiem, Fracture du verre et heterogeneities a l'echelle submicronique, These, Universite Paris VI, 1998

[11] P.Daqnier, B.Nghiem, E.Bauchand, F.Creuzet, Physical Review Letters, 78 (1997) 1062

[12] J.Schmelzer, J.Non. Cryst. Solids 183 (1995) 215-233