Numerical Simulation Studies of Peripheral Roughening in a Monolayer

Recently Kołaczkiewicz and Bauer[1] argued that an experimental realization of a spin model by Abraham and Smith[2] is obtained by a monolayer of an fcc metal (for instance Au) on a bcc substrate (for instance W). In this 2D model the roughening temperature T_R of the periphery can be greater than zero provided that the peripheral bonds are weaker by a factor α than the interior bonds (for equal bond strengths $T_R=0$). In the interpretation of the experiment in Ref. 1, the roughening temperature is claimed to increase from 0 to the critical temperature as α decreases from 1 to 0. Therefore, the peripheral roughness increases with increasing α, which is claimed to be in accordance with the model of Abraham. However, this interpretation is clearly counterintuitive since one expects that, as α increases, the peripheral atoms are bonded more tightly and therefore the roughness decreases. Moreover, it has been shown earlier[3] that the essential feature of the transition in the Abraham model is the presence of a "hard wall" where the interfacial spins are pinned. This hard wall is not present in the present case. In the present numerical study we show that in accordance with intuitive ideas, the roughness increases with decreasing α, which is contrary to the claims of Ref. 1.

We have solved, using molecular-dynamics simulation, the model, i.e., a 487-particle movable layer on an infinite bcc substrate, which according to Ref. 1 applies to Au on W(110). In this model, the forces J_1 between the boundary and the interior Au atoms are weaker than the forces J between the interior Au atoms themselves i.e., $J_1=\alpha J$ with $\alpha<1$. Under ordinary conditions (i.e., $\alpha=1$) the overlayer crystallizes on a 2D triangular lattice, corresponding to a (111) fcc plane. The ratio of the triangular to bcc lattice parameters is chosen to be equal to the one that gives a minimum of the epitaxial energies[4] (1.33) and is close to the ratio of Au-W lattice parameters (1.291). The overlayer and overlayer-substrate particles interact via ordinary Lennard-Jones potentials. In order to stabilize the triangular overlayer crystal on the bcc substrate the overlayer-overlayer atom interaction is $\frac{7}{2}$ of the overlayer-substrate atom interaction.

Figure 1 shows the number of peripheral atoms N_s as a function of α for two different temperatures. Clearly N_s increases with decreasing α, diverging as α approaches a small value. In addition, the higher-temperature curve shows a rougher surface in accordance with intuitive expectations.

We conclude that the interpretation of the experiments of Ref. 1 has to be modified. In particular, the manner in which alteration of the peripheral bonds in the Abraham model transfers to the monolayer model has to be reevaluated.

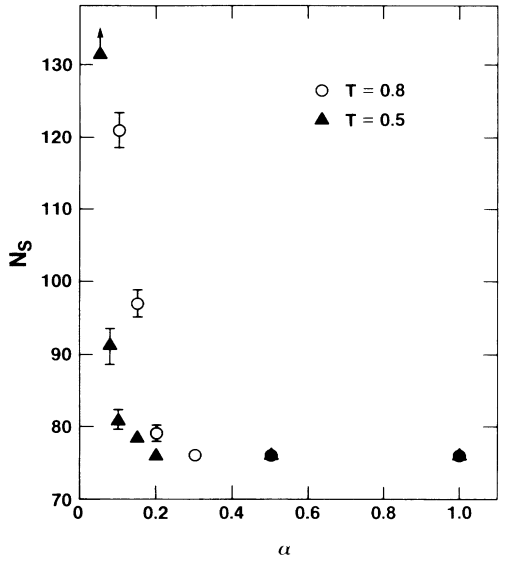

FIG. 1. Dependence of N_s on α for two temperatures. Note that the surface is rougher for lower α and higher temperatures.

This work was supported in part by the U.S. Department of Energy, Basic Energy Sciences Program– Materials Sciences, under Contract No. W-31-109-ENG-38, the Catholic University of Chile, the Fondecyt-Conicyt, Programme des Nations Unies por le Developpement, the Organization of American States, the National Science Foundation–American Physical Society Latin American Assistance Program, and IBM Chile for computer time in the initial stages of this work.

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(Received 9 July 1986)
PACS numbers: 64.70.Kb, 68.35.Md, 73.30.+y, 82.65.Dp

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