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Avalanche in Adhesion at bcc Metal Interfaces

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Abstract: It has been shown that as two metal surfaces approach each other the surfaces can avalanche together when the rigid interfacial spacing falls below a critical distance. We examine this phenomenon for the bcc metals Fe and W using the Equivalent Crystal Theory. We also examine the effect of loss of registry between the two surfaces. The avalanche is inhibited when the two surfaces are sufficiently far out of registry and when only a few surface layers are allowed to relax. As the relaxing slabs get thicker a sharp avalanche reappears.

Keywords: Surfaces, interfaces, adhesion, avalanche, structure, energy, simulation

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I. Introduction

Recent simulations[1-4] have shown that approaching solid surfaces can jump across and close the interfacial gap even when the initial interfacial separation is much larger than the bulk interplanar spacing. Smith *et al.*,[2] studied the (100) interface of Ni using the Equivalent Crystal Theory (ECT)[5,6] based on the universal binding energy relation (UBER).[7] At each value of the rigid interfacial spacing, d_R, a number, n, of planes parallel to the interface were allowed to relax, *i. e.* move normal to the interface in order to minimize the total energy. When d_R fell below some critical value, d_R^{crit}, the surface atomic layers jumped across the interfacial gap and came together. This jumping across, or avalanche, was accompanied by a discontinuous drop in adhesive energy. The elastic strain was gradually relieved as d_R was decreased

farther. The post-avalanche variation of the adhesive energy with d_R was nearly parabolic, quite different from the behaviour of the energy in the case of rigid adhesion which followed the UBER.[9] As n increased, d_R^{crit} also increased.[2] Smith *et al.*[2] argued that as $n \rightarrow \infty$, $d_R^{crit} \sim ln\, n$ and the discontinuity in the energy approaches the surface energy of the particular surface.

Smith *et al.*[2] indicated some circumstances under which avalanche may be inhibited. Among other things, they suggested that a lack of registry across the interface may prevent, or severely inhibit avalanche. In a subsequent study of avalanche Good *et al.*[4] reported that for Ni (001) in the event of a total loss of registry - so that atoms on either side of the interface come down on top of each other - avalanche is severely inhibited. In this case there is no sharp drop in the energy but there is a significant, though rounded, avalanche-like change in the interlayer spacings. That study[4] allowed no more than three surface layers on either side to relax and the authors noted that as the number of relaxing layers increased the changes in the interlayer spacings appeared to get sharper.

In this paper we present a study of avalanche at the (110) interfaces of the bcc metals Fe and W. We also present here a study of the effect of registry on avalanche at the Fe(110) interface. In the next section we present a brief review of the simulation procedure while in Section III we present and discuss our results. Finally, we summarise the study in Section IV.

II. Simulation procedure

In these simulations we have used the Equivalent Crystal Theory[5,6] (ECT) to compute the energies of the system. Though this method has been described in detail elsewhere, we present here a very brief review of the essentials. ECT normally expresses the energy of a collection of atoms as a sum over individual atomic contributions. Each atomic contribution comprises four different terms. The first of these depends basically on the local density in the neighbourhood of the atom in question and is usually the largest single contribution to the surface or interface energy. The second term accounts for local variations in nearest-neighbour distances. The other two terms depend on changes in bond angles and account for shear-like distortions. ECT has been shown to give accurate surface energies and relaxations for several materials.[5,6,8,11] It has also been shown[11] that the bond-angle-dependent terms contribute little to the relaxation energies of metal surfaces. Hence, we have neglected the last two terms of the ECT energy expression.

Here we have considered planar relaxations only. At each value of d_R the energy of the system - two semi-infinite solids with parallel surfaces either in or out of registry - was minimized with respect to the interlayer spacings using a zero-temperature Monte Carlo procedure. Since we were interested in studying the evolution of a local minimum we have not used the full Metropolis algorithm.[10] Effects of finite temperature and in-plane reconstruction will be discussed in a later publication. The variations in interlayer spacings were assumed to be symmetric about the interface. As a result the energies presented here are half of the total energies of adhesion and the depth of the energy well is the surface energy of the appropriate metal surface.

III. Results

The variation of relaxed binding energy with d_R for the case with the approaching surfaces in perfect registry, is shown in Figs. 1 and 2 for the (110) interfaces of Fe and W, respectively. The sudden drop in the energy upon avalanche is clearly evident.

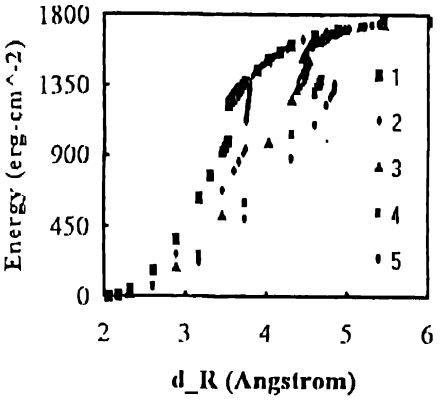

Fig. 1. Plots of relaxed energy *vs.* d_R, for the Fe(110) interface in registry.

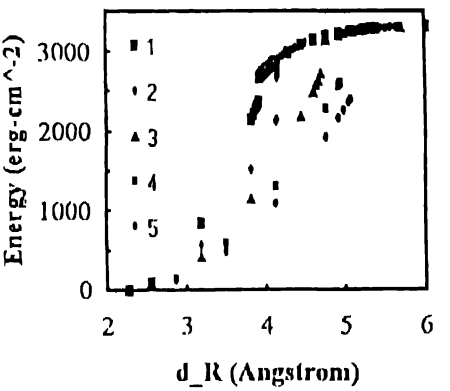

Fig. 2. Plots of relaxed energy *vs.* d_R, for the W(110) interface in registry.

The physical transformation associated with this drop in energy is seen clearly in Figs. 3 and 4 which show - for the Fe and W (110) interfaces, respectively, (in perfect registry) and different numbers of relaxing layers as indicated - plots of the relaxed interfacial separation as a function of d_R. At large values of d_R, when the surfaces are essentially isolated and not interacting, the relaxed interfacial separation is slightly greater than d_R. This means that each surface layer relaxes in toward the bulk – a phenomenon known from experiment as well as theory.[5,6,8,11] As d_R decreases, there is a gradual reduction in the inward relaxation of the surface layer. At a certain "critical" value of d_R, however, there is a sudden drop in the interfacial separation as the surface layers leave their respective slabs and come together in the center.

We have plotted in Figs. 6 and 7 the critical value of d_R for avalanche, d_R^{crit}, against n, the number of relaxing layers. We have plotted a least squares fit to a logarithmic function to the data. The fitted function is indicated on each graph.

So far the two approaching surfaces have been in perfect registry so that when d_R is reduced to the equilibrium interplanar spacing, d_{110}, the two slabs join to make a complete solid and the interface disappears. We now present results for the Fe(110) interface when the two approaching surfaces are not in registry. In what follows, starting from the case of perfect registry, one half solid has been shifted relative to the other by small amounts in a direction parallel to the interface.

Good *et al.*[4] had presented preliminary results for avalanche in the case of out-of-registry approach at the Ni(001) interface. There the shift had been such that

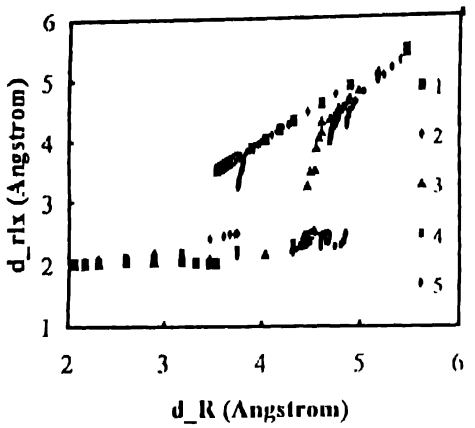

Fig. 3. Plots of relaxed interfacial separation *vs.* d_R for the Fe(110) interface.

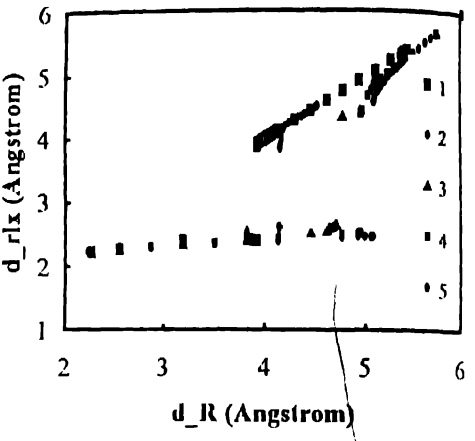

Fig. 4. Plots of relaxed interfacial separation *vs*, d_R for the W(110) interface..

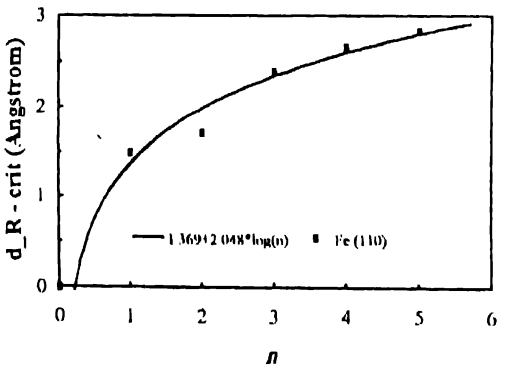

Fig. 5. Values of d_R^{crit} *vs.* n plotted for the Fe(110) interface. The solid line shows a least-squares fit to a logarithmic function.

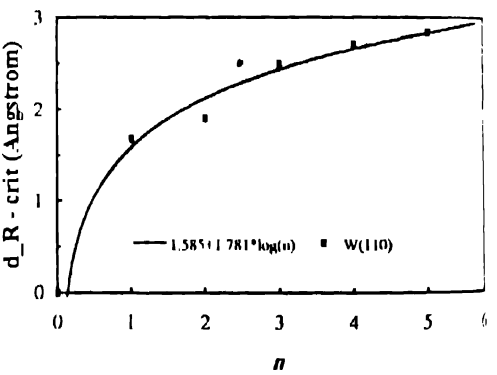

Fig. 6. Values of d_R^{crit} *vs.* n plotted for the W(110) interface. The solid line shows a least-squares fit to a logarithmic function.

atoms on one surface layer came down on top of atoms of the other as d_R was reduced to zero. This "total" loss of registry strongly inhibited avalanche when upto three layers were allowed to relax. However, the rounded, gradual transitions grew sharper as the number, n, of relaxing layers increased. We have investigated this phenomenon for the Fe(110) interface only as the results for W(110) are expected to be essentially similar to those for Fe(110).

Figures 7 through 10 show plots of relaxed interfacial spacing and relaxed adhesive energy, respectively, against d_R for out-of-registry Fe(110) interfaces with one and five layers relaxing. Results are shown for two different amounts of shift, as

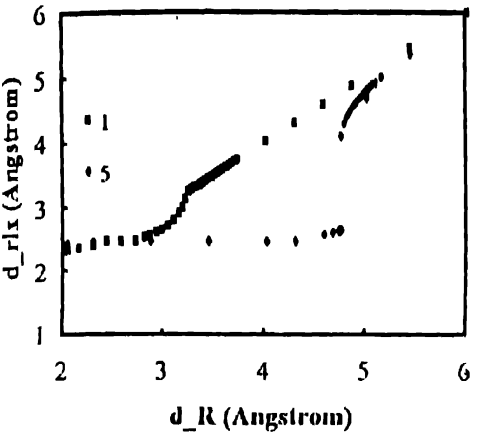

Fig. 7. Plots of relaxed interfacial separation *vs.* d_R for an out-of-registry Fe(110) interface. One surface has been shifted relative to the other in the $(\bar{1}10)$ direction by $\frac{1}{2}d_{110}$. Results shown are for cases with 1 and 5 surface layers relaxing.

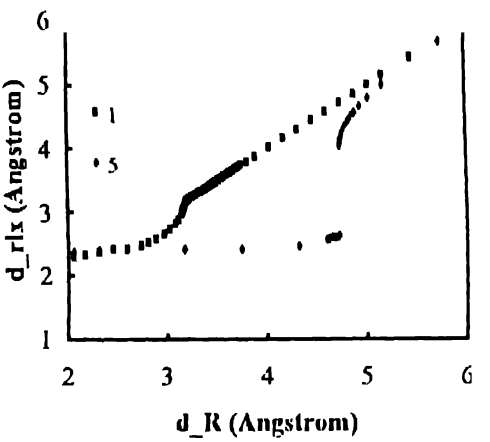

Fig. 8. Plots of relaxed interfacial separation *vs.* d_R for an out-of-registry Fe(110) interface. One surface has been shifted relative to the other in the $(\bar{1}10)$ direction by $\frac{3}{4}d_{110}$. Results shown are for cases with 1 and 5 surface layers relaxing.

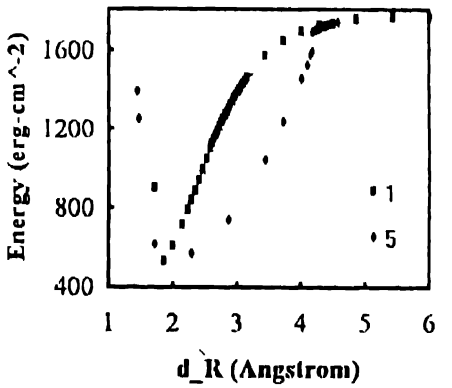

Fig. 9. Relaxed energy *vs.* d_R plotted for an out-of-registry Fe(110) interface. One surface has been shifted relative to the other in the $(\bar{1}10)$ direction by $\frac{1}{2}d_{110}$. Results shown are for cases with 1 and 5 surface layers relaxing.

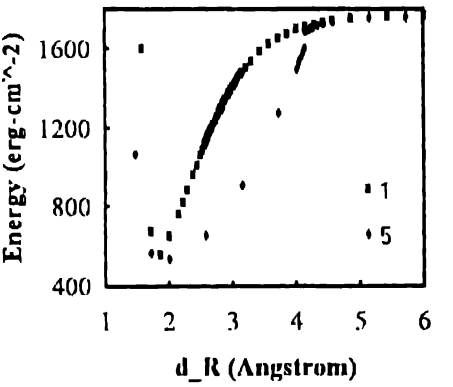

Fig. 10. Relaxed energy *vs.* d_R plotted for an out-of-registry Fe(110) interface. One surface has been shifted relative to the other in the $(\bar{1}10)$ direction by $\frac{3}{4}d_{110}$. Results shown are for cases with 1 and 5 surface layers relaxing.

labeled, in the $(1\bar{1}0)$ direction. We can see that there appears to be no sharp drop in energy associated with avalanche when only one surface layer is allowed to relax.

However, upon allowing more layers to relax we do see a sharp discontinuity in the energy associated with avalanche. At the same value of d_R the relaxed interfacial separation shows a sharp discontinuity in its derivative. Such a discontinuity is also seen for the case where only one layer is allowed to relax. This indicates that a sort of avalanche occurs even when the approaching surfaces are out of registry provided a sufficient number of layers are allowed to relax. However, it is clear that the drop in energy associated with avalanche is much smaller in this case.

IV. Discussion and Summary

Avalanche can be understood as a competition between the attractive interaction of a surface layer with other layers in the same slab, and with the surface layers across the interface in the other slab. At large d_R a surface layer interacts only with layers in the same slab. Hence, it moves in toward the bulk of the slab. As d_R decreases, the surface layer begins to experience an attraction to the layers across the interface. Ultimately, at d_R^{crit}, forming bonds across the interface lowers the energy enough to offset the increase in energy due to stretching of the bonds with its neighbouring bulk layers. This is when avalanche occurs.

The inhibition of avalanche in the out-of-registry case, at least for thin slabs, can be understood by looking at the surface geometries. In the in-registry case, each (110) surface atom is bonded to two atoms in the neighbouring bulk layer, four atoms in the same layer, and, for small enough d_R two atoms across the interface. Thus the interaction with the two atoms across the interface will have a weight equal to that of interactions with atoms in the neighbouring substrate layer as long as perfect registry is maintained. In the out-of-registry case a surface atom is bonded to the same number of atoms as before within the same slab but In the other slab there is only one "nearest-neighbour" atom. As the slabs approach each other, the interaction across the interface is substantially weaker than in the in-registry case. There are two other atoms in the surface plane across the interface which might be called "secondary" near neighbours rather than second-nearest neighbours. The interactions with these will be strongly screened, especially at small values of d_R. So these cannot compensate for the decreased coordination across the interface. This is what inhibits the sharp avalanche in the out-of-registry case.

As n increases a significant amount of energy can be gained by relaxing the deeper layers outward. When the surface layer moves out in order to "gain" coordination the energy cost for stretching the bonds with the substrate can be minimized by distributing the "strain" over several interlayer bonds. This is why avalanche returns when n increases.

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