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Catalytic reactions on mono- and bi-metallic surfaces

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Abstract. Catalytic reactions such as A(gas) + B(gas) $\Rightarrow$ AB(inert) on single- and binary-crystal surfaces are simulated using the Monte Carlo method. It is shown that at the steady reactive state the critical concentrations of the reactants are analytical functions of their sticking coefficients.

A catalytic reaction depends on a number of intrinsic and extrinsic parameters [1–3]. Of these, the sticking probability of the reacting agents on a given surface is one of the most important. Hence, we propose to study the behaviour of the critical concentrations (at the steady reactive state) of the reactants as functions of the sticking coefficients. We consider a square lattice of 40×40 lattice sites with periodic boundary conditions. We start with an empty lattice and choose an empty site randomly. The choice of the atom for adsorption is also made randomly. A number between zero and one is chosen randomly. If this number is smaller than the sticking coefficient of the atom concerned, then (and only then) the adsorption takes place. A and B on nearest-neighbour sites immediately react to form AB which immediately desorbs. For a given value of the sticking coefficients of A and B we try to find a critical concentration X_{cA} of A in the reservoir such that the surface is not 'poisoned' by either A or B.

In the case of the single-crystal surface, the results obtained through simulation obey an analytical relation:

$$X_{cA} = S_A/(S_A + S_B)$$

where S_A (S_B) is the sticking coefficient of A (B). A particular point (i.e. $X_{cA} = 0.5$ when $S_A = S_B = 1$) of this general expression has already been studied by many authors [4, 5].

For a bi-metallic surface composed of two metals a and b of equal concentration, we obtain some beautifully symmetric curves. Figure 1 presents X_{cA} versus S_{Aa} for some fixed values of S_{Bb}, where S_{Aa} (S_{Bb}) is the sticking coefficient of atom A (B) on the metal site a (b). From observing the symmetry of these curves and the asymptotic behaviour at the end points, one obtains an analytical expression:

$$X_{cA} = \tfrac{1}{2} - \tfrac{1}{2}\frac{\sqrt{[S_{Aa}(1 - S_{Bb})]} - \sqrt{[S_{Bb}(1 - S_{Aa})]}}{\sqrt{[S_{Aa}(1 - S_{Bb})]} + \sqrt{[S_{Bb}(1 - S_{Aa})]}}.$$

It is possible to extend the use of the sticking coefficient to small molecules such as CO and O_2 to study the oxidation of CO. Work along these lines is in progress.

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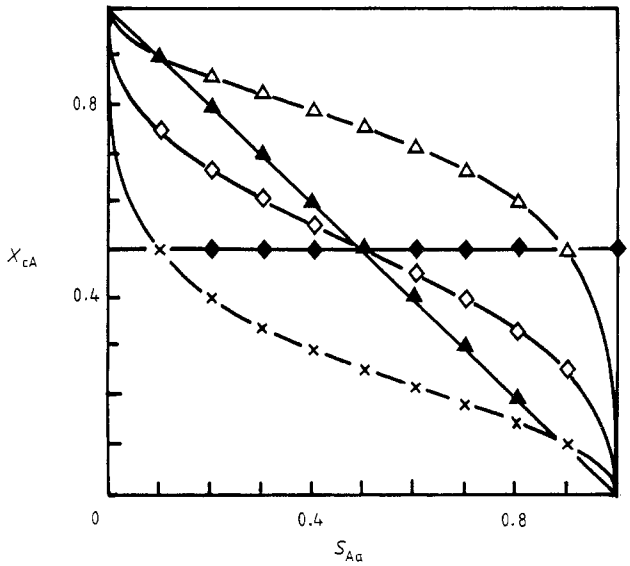

Figure 1. X_{cA} versus S_{Aa} for fixed values of S_{Bb}. ×, $S_{Bb} = 0.1$; ◇, $S_{Bb} = 0.5$; △, $S_{Bb} = 0.9$; ◆, $S_{Bb} = S_{Aa}$ and ▲, $S_{Bb} = 1 - S_{Aa}$.

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