NO+CO SURFACE–REACTION MODEL

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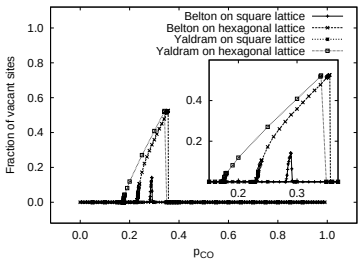
Monte Carlo simulations of the CO+NO reaction supported on surface were carried out using the mechanism proposed by Belton et al., given by:

(1)	CO(g)+$\star$	$\rightarrow$	CO(a)	(2)	NO(g)+$\star$	$\rightarrow$	NO(a)
(3)	NO(a)+$\star$	$\rightarrow$	N(a)+O(a)	(4)	N(a)+N(a)	$\rightarrow$	N_2(g)+2$\star$
(5)	NO(a)+N(a)	$\rightarrow$	N_2O(g)+2$\star$	(6)	CO(a)+O(a)	$\rightarrow$	CO_2(g)+2$\star$

The results have been analysed and compared with previous studies based on the scheme presented by Yaldram & Kahn, which does not allow the existence of NO on the surface as a monomer (so it must be adsorbed onto a couple of empty nearest-neighbours sites) and does not contain reaction (5).
Both mechanisms behave in a similar way on a hexagonal lattice. A steady reactive window (SRW) is observed, delimited for two values of y_{CO} (y_1 and y_2), the molar fraction of CO in the gas phase. The SRW is identified by the existence of vacant sites on the lattice. At y_1, a continuous phase transition takes place, whereas for y_2 there is a first-order transition, characterized by a sudden change in the fraction of vacant sites on the surface.
Our simulations for a square lattice show the existence of a narrow SRW (see figure), not predicted for the Yaldram model. In this case, the nature of the phase transition changes, and it is of continuous type for both points.



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