

## 6.4: Examples - Surface Structures

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This section provides worked exercises in the classification of surface structures using both Wood's notation and matrix notation, and in the determination of surface coverages.

*Note - all surface coverages discussed in this section are defined in the conventional surface science manner, by reference to the number density of the underlying layer of surface atoms of the substrate*

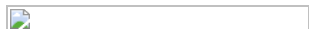
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### Structure #1



- How would this centred structure observed on fcc(100) surfaces be described using Wood's notation ?
  - What is the coverage of adsorbate for this surface structure ?
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### Structure #2



- How would this structure on the fcc(100) surface be described using Wood's notation ?
- What is the coverage of adsorbate for this surface structure ?

**Note** - in this instance the structure illustrated is but one of two equivalent domains - related by the symmetry of the substrate. The second domain is shown below.



It differs from the first only in that the closely-packed rows of the adsorbate now run at 90 degrees to their direction in the first domain. Patches of this domain structure would exist on the surface with statistically-equal probability to the other domain. It

obviously corresponds to the same adsorbate coverage and must possess identical properties (electronic, thermodynamic & reactivity).

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### Structure #3



- ⇒ How would this adsorbate structure on the  $fcc(110)$  surface be described using Wood's notation ?
  - ⇒ What is the coverage of adsorbate for this surface structure ?
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### Structure #4



- ⇒ How might this adsorbate structure on the  $fcc(111)$  surface be described using Wood's notation ?
  - ⇒ What is the coverage of adsorbate for this surface structure ?
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### Structure #5



This shows an alloy surface layer on an  $fcc(111)$  substrate - such a layer might be formed by two metals which alloy if one is evaporated onto a (111) single crystal surface of the other.

- ⇒ How might this superstructure be described using Wood's notation ?
  - ⇒ What are the relative concentrations of the two elements in the surface layer ( specified as the ratio of A:B atoms ) ?
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## Structure #6

The diagram below shows a "coadsorption" structure in which adsorption of two different species has led to the formation of an ordered surface layer containing both species - such structures ( albeit more complicated than the one shown ) are known for a number of pairs of adsorbates on a variety of surfaces e.g. benzene / CO - Rh(111)



The driving force for the formation of such structures may be an attractive dipole-dipole force between the two different adsorbed species (this might occur if, for example, one acts as an electron donor whereas the other acts as an electron acceptor on the substrate concerned).

— How would this structure be classified using Wood's notation ?

— What are the relative concentrations of the two species in the coadsorption structure ?

## Structure #7

The diagram below shows a molecular adsorption structure in which a diatomic molecule is bonded terminally to substrate atoms but is inclined to the surface normal. This particular structure has not been observed but similar structures involving a periodic tilting of the molecular axis have been discovered, e.g. CO / Pd(110) .



— How would this structure be classified using Wood's notation ?

## Summary

The structures of ordered adsorbate overlayers may be defined by specifying the adsorbate unit cell in terms of the ideal substrate unit cell - in many cases, such as the examples given, this can be done using the simple Wood's notation and this is the common practice. In more difficult cases it may be necessary to use matrix notation.

In all the examples studied :

1. the overlayers were simple structures in which the adsorbate unit cell dimensions corresponded to one of the atom-atom spacings in the underlying substrate structure ; this is generally the case for adsorbed overlayers of gaseous molecules. More complex "coincidence" and "incommensurate" structures are commonplace when the overlayer consists of one or more atomic layers of a distinct chemical compound e.g. oxide overlayers on metals.
2. it was assumed that the underlying substrate structure was undisturbed by the adsorption of species on the surface. Whilst such distortions may generally be small, this is far from always being the case and a number of examples involving adsorbate-induced reconstruction of the topmost layer of substrate atoms have now been well documented ( e.g. Ni(100) c(2x2)-C ).

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