PAC : application

www. hyperfinecourse .org

impurities at surfaces

Hyperfine interaction methods allow to study the behaviour of a single impurity atom on a surface:

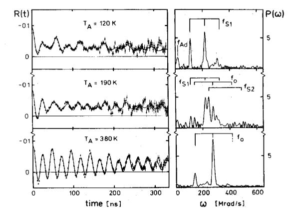

Fig. 5.22 PAC spectra along with their Fourier transforms for ^{111}In on stepped Ag(100) for three different annealing temperatures (annealing time 15 minutes, measuring temperature 77 K). The solid lines were fitted to the experimental points by Eq. (5.41).

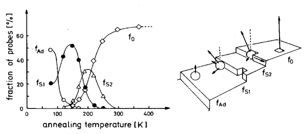

Fig. 5.23 Left side: Fraction of indium probes with different electric field gradients on stepped Ag(100) as a function of annealing temperature. Right side: Surface site model for indium probes suggested by the experimental parameters.

Source: Nuclear Condensed Matter Physics
G. Schatz and A. Weidinger

T. Klas et al., Surf. Science 216 (1989) 270-302
G. Krausch et al., Hyp. Int. 78 (1993) 261-280
H. Haas, Z. Naturforsch. 50a (1994) 407-417
… and many others

2

impurities at surfaces

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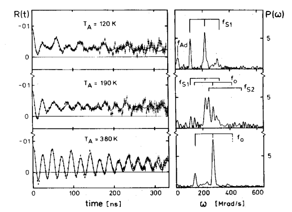

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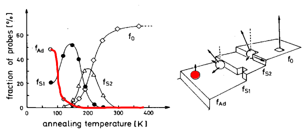

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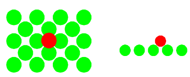

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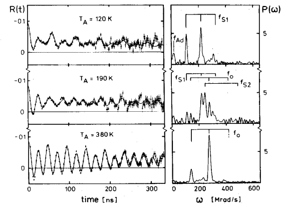

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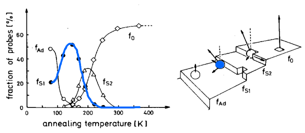

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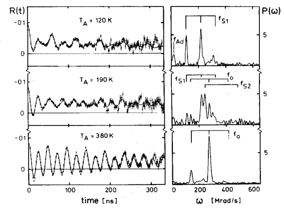

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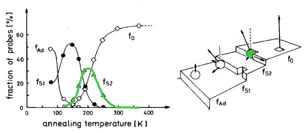

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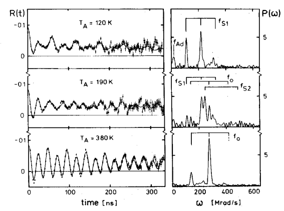

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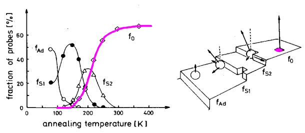

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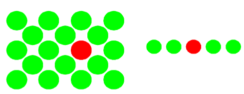

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impurities at surfaces

	Ni	Cu	Pd	Ag
(100) terrace	8.2	10.3	8.2	7.5
(100) adatom	2.8 / 0.3	0.8	2.8	0.3
(110) terrace	--	7.9	--	7.0
(110) adatom	--	--	--	--
(111) terrace	11.5 / 12.3	10.2	10.2	8.6
(111) adatom	1.0	--	0.4	--

Practical rule :
- large V_{zz} = terrace site
- small V_{zz} = adatom site

WHY ?
And (110) ?

Ni 28	Cu 29
Pd 46	Ag 47

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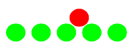
impurities at surfaces

(100) terrace

(100) adatom



	|Exp|	Calc
Ni	8.2	8.6
Cu	10.3	9.9
Pd	8.2	9.1
Ag	7.5	8.5
Ni	2.8/0.3	1.9
Cu	0.8	-2.0
Pd	2.8	3.4
Ag	0.3	0.4

V_{zz} large

V_{zz} small

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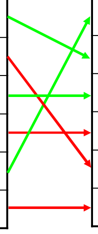
impurities at surfaces

Cd on Pd (unrelaxed) as a model system

NN		V_{zz} (calc)
8	(100) Terrace	8.8
4	(100) Adatom	2.8
7	(110) Terrace	8.1
5	(110) Adatom	4.2
9	(111) Terrace	9.6
3	(111) Adatom	-0.8



V_{zz} (calc)		NN
9.6	(111) Terrace	9
8.8	(100) Terrace	8
8.1	(110) Terrace	7
4.2	(110) Adatom	5
2.8	(100) Adatom	4
-0.8	(111) Adatom	3

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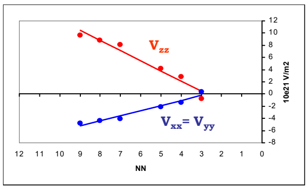
impurities at surfaces

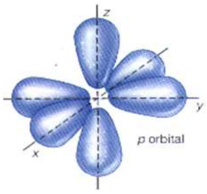
Cd on Pd (unrelaxed) as a model system



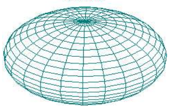
V_{zz} (calc)		NN
9.6	(111) Terrace	9
8.8	(100) Terrace	8
8.1	(110) Terrace	7
4.2	(110) Adatom	5
2.8	(100) Adatom	4
-0.8	(111) Adatom	3

(note: didactical short-cut for V_{xx} and V_{yy} on (110) surfaces)

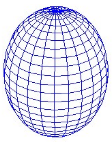
impurities at surfaces



$$V_{zz} \propto \frac{p_x + p_y}{2} - p_z$$

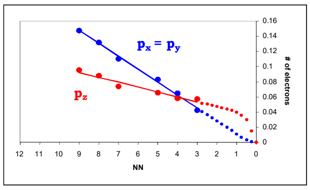


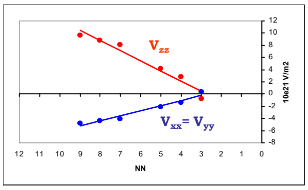
$V_{zz} > 0$



$V_{zz} < 0$

impurities at surfaces





	NN	Horizontal	Vertical
(111) Terrace	9	6	3
(100) Terrace	8	4	4
(110) Terrace	7	2	5
(110) Adatom	5	0	5
(100) Adatom	4	0	4
(111) Adatom	3	0	3
Free atom	0	0	0

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