PHY 752 Solid State Physics
11-11:50 AM MWF Olin 107

Plan for Lecture 30:

- Surface properties of solids (some material in Marder Chap. 4, 19, 23)
  - Geometric and electronic structures of surfaces
  - Work function
  - Photoemission

21	Wed: 03/18/2015	Chap. 16	Electron Transport	#20	03/20/2015
22	Fri: 03/20/2015	Chap. 16	Electron Transport	#21	03/23/2015
23	Mon: 03/23/2015	Chap. 17	Electron Transport	#22	03/25/2015
24	Wed: 03/25/2015	Chap. 17 & 18	Electron Transport		
25	Fri: 03/27/2015	Chap. 18	Microscopic picture of transport	#23	03/30/2015
26	Mon: 03/30/2015	Chap. 19	Semiconductor devices	#24	04/01/2015
27	Wed: 04/01/2015	Chap. 20	Models of dielectric functions	#25	04/06/2015
	Fri: 04/03/2015	Good Friday	No class		
28	Mon: 04/06/2015	Chap. 21	Optical properties of solids	#26	04/08/2015
29	Wed: 04/08/2015	Chap. 22	Modern theory of polorization	#27	04/10/2015
30	Fri: 04/10/2015		Surface properties of solids	#28	04/13/2015
31	Mon: 04/13/2015				04/15/2015
32	Wed: 04/15/2015				04/17/2015
33	Fri: 04/17/2015				04/20/2015
34	Mon: 04/20/2015				
35	Wed: 04/22/2015				
36	Fri: 04/24/2015				
	Mon: 04/27/2015		Presentations I		
	Wed: 04/29/2015		Presentations II		
	Fri: 05/01/2015		Presentations III & Take home exam		

Surface effects in solids

Some material is taken from the review article:

Rep. Prog. Phys., Vol. 45, 1982. Printed in Great Britain pages 223-284

Surface electronic structure

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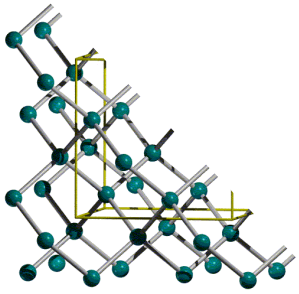
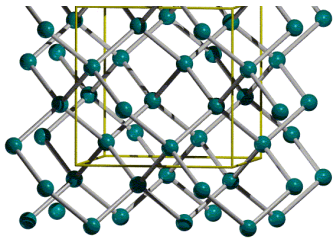




What happens when crystal is cleaved?

- Potential barrier between inside of crystal and vacuum – work function
- Crystal loses periodicity in cleavage direction (band smearing)
- Possibility of surface states
- Possibility of image potential states

Projection of effective potential near surface

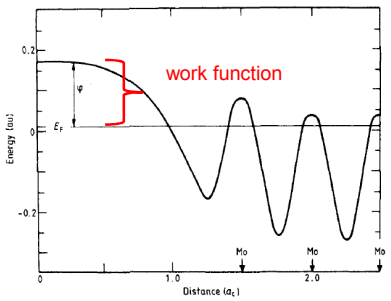
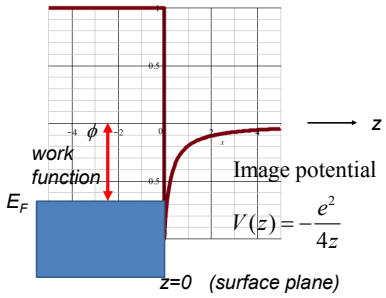


Figure 1. Potential at Mo (001) surface (averaged parallel to the surface). Arrows mark the positions of atomic layers and φ is the work function (Kerker *et al* 1978).

Model of interface:



Bloch symmetry due to surface

$\mathbf{k}=\mathbf{k}_{\parallel}+k_z\hat{\mathbf{z}}$ ← no longer periodic

surface bands

bulk bands

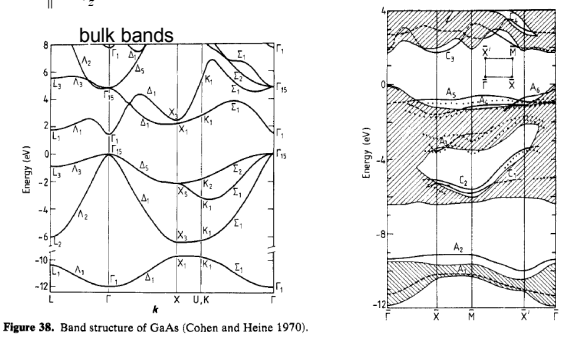


Figure 38. Band structure of GaAs (Cohen and Heine 1970).

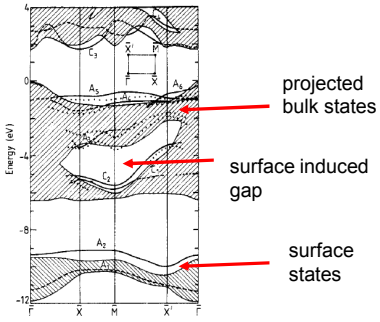


Figure 41. Surface states and resonances on relaxed GaAs (110) as a function of ***K*** in surface Brillouin zone. The shaded area shows the projected bulk GaAs bands. The full curves show the calculated results (Chelikowsky and Cohen 1979) and the dotted curves experimental results (Huijser *et al* 1978).

Relaxation of surface atoms – example Ni (001)

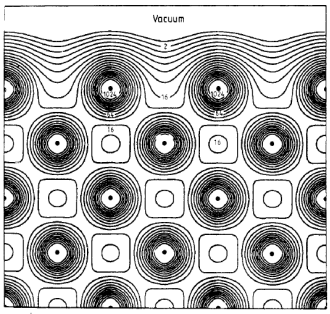


Figure 29. Contours of charge density at Ni (001) surface (Arlinghaus *et al* 1980).

Electronic structure calculation for slab

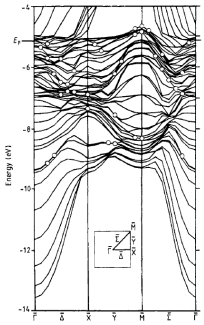


Figure 30. Energies of states in Ni (001) slab as a function of ***K***. Circles indicate surface states/resonances (Arlinghaus *et al* 1980).

Surface reconstruction – Si (001)

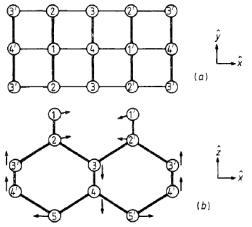


Figure 35. Si (001) (2×1) reconstruction: (*a*) top view; (*b*) side view (Chadi 1979a).

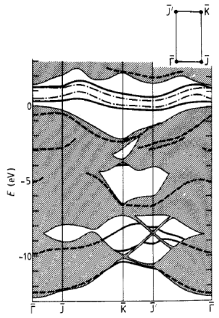


Figure 36. Surface states and resonances in Si (001) asymmetric dimer (2×1) reconstruction, as a function of ***K*** in surface Brillouin zone. The shaded area shows the projected bulk Si bands. The chain curve shows surface states for a symmetric dimer reconstruction (Ihm *et al* 1980).

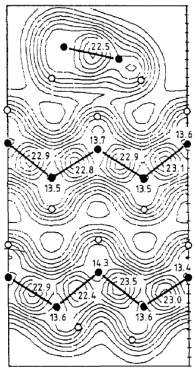
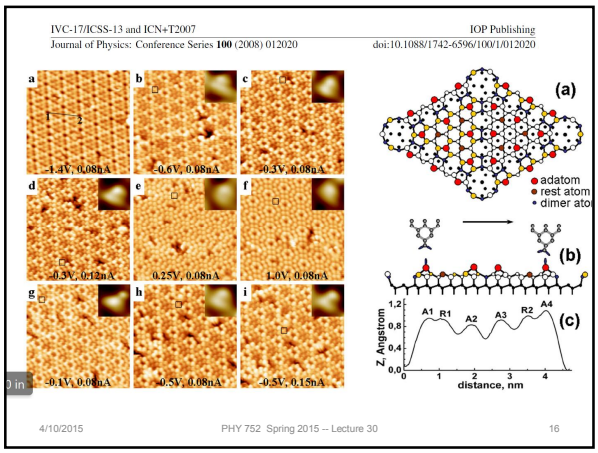
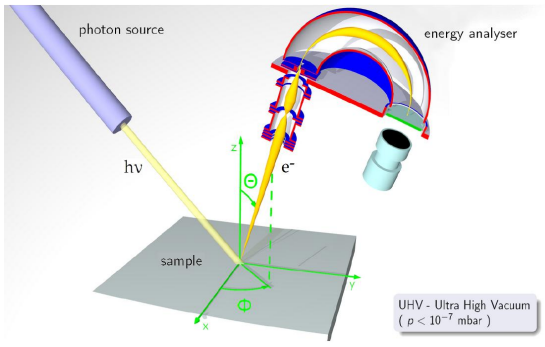


Figure 37. Contours of charge density at (2×1) reconstructed Si (001) surface (Ihm *et al* 1980).



Photoemission measurements (materials from Matthias Kreier of Humbolt University)



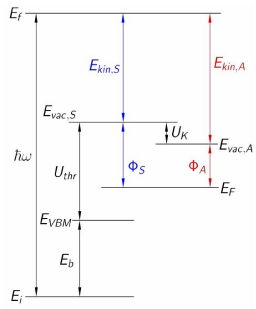
Transition rate from Fermi Golden Rule

$$\omega_{fi} = \frac{2\pi}{\hbar}|\langle\Phi_f|H_{WW}|\Phi_i\rangle|^2\delta(E_f - E_i - \hbar\omega)$$

$$H_{WW} = \frac{e}{2mc}\vec{A}\cdot\vec{p}$$

Energy and momentum conservation

$$E_f = E_i + \hbar\omega \qquad \vec{k}_i = \vec{k}_f$$



E_i	energy of initial state
E_f	energy of final state
E_{VBM}	valence band maximum
$E_{vac,S}$	vacuum level of sample
$E_{vac,A}$	vacuum level of analyser
$\hbar\omega$	photon energy
U_b	binding energy
E_{thr}	threshold of photo emission
$E_{kin,S}$	kinetic energy of eletrons at the sample
$E_{kin,A}$	kinetic energy of eletrons at analyser
U_K	contact potential
Φ_S	work function of sample
Φ_A	work function of analyser
E_F	Fermi energy