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SELFCONSISTENT CALCULATIONS OF THE ELECTRONIC PROPERTIES OF SIMPLE METAL SURFACES

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Abstract: The surfaces of Al and Na are simple systems but interesting features are present, like surface states and image resonances. We use the Weighted Density Approximation (WDA), which accounts for image effects, in the description of their electronic properties.

1. Introduction

Image effects at surfaces are very important : tunneling current, atom-surface interaction, lifetimes of excited atomic states near a surface, are strongly influenced by image forces, which in density functional theory cannot be described within the LDA. The aim of this work is to apply a non local scheme, the WDA, previously used in the jellium model[1], to the surfaces of some simple metals.

2. The model

The WDA was introduced by Gunnarsson and Jones[2] and used by several authors in the calculation of electronic properties of atoms, solids, surfaces[3]. We point out that in the limit of very large distances from the surface, our exchange-correlation hole is equivalent, at the lowest order, to the classical image charge, and this is the reason why WDA gives the image behaviour. We use a laterally averaged pseudopotential and perform one-dimensional selfconsistent calculations, using a repeated-cell method in the z direction perpendicular to the surface. In this way the different surfaces are characterized by the different stacking of the atomic planes. This model accounts very well for surface electronic properties, like work function and image effects, moreover it describes simply but with good accuracy the crystal potential in the z direction in all the cases in which the band structure shows a quasi-free electron dispersion along the direction parallel to the surface. This is confirmed by the fact that the model reproduces the band structure in k_z of Al and Na correctly.

3. Results

Work function values (see table 1) are in excellent agreement with the experimental data[4]. We find surface states in Na(110) at 0.69 eV above the Fermi level, just on the upper edge of the band. In Al(100) a surface state is located 2.92 eV below E_F, 0.36 eV above the bottom of the inner gap at $\mathbf{k}_{||} = 0$. Similar results were found by other authors[5] through tridimensional calculations. The corrispondent wavefunction shows how in the case

of Na(110) the decay into the the bulk is quite slow, in fact the state lies just above the top of the band, so the imaginary part of its wavevector is small. The correct description of the selfconsistent potential is important in characterizing this states as a decaying state and not simply as a resonances, in spite of their slow decays into the bulk.

Another interesting feature is represented by the presence of *image states*, whose existence is due to the image behaviour of the effective potential outside the surface; they have been detected in a large number of metals. To calculate their wavefunctions it is necessary to describe correctly as well the band structure above E_F as the selfconsistent saturation of the image potential for the different surfaces. It is important to distinguish two cases, depending on the fact that the values of the quasi-Rydberg series of the image state energies lies or does not lie in a gap of the projected band structure. In the first case the internal wave is evanescent, and there is only one E value where the matching of the internal and external wave is allowed; this happens for several transition and noble metals surfaces, and we call these states "pure image states". Otherwise if the Rydberg series corresponds to a continuum of bulk states, for each energy E there is a wave matching with an external wavefunction, giving what we call a "resonant image state". Experimentally the two kinds of image states show quite different features; pure image states give sharp peaks, while resonant states give broad structures in the spectra. The latter is the case of Al(111)[6], in agreement with our calculations. Also in Al(100) and Na(110) there is a continuum of states below the vacuum level. The mean energy of these wide resonances can be calculated by weighting each energy by the square modulus integral of the wavefunction in the vacuum region. The results are shown in table 2, where E_n is the average binding energy of the n-th resonance relative to the vacuum level. These resonances in Al(111) are really broadened and they must be compared[6] with a single structure (0.55 eV) seen in inverse photoemission where contributions of both $n = 1$ and $n = 2$ image resonances are present.

table 1		Φ (eV)	exp.
	Al(111)	4.19	4.24
	Al(100)	4.23	4.30
	Na(110)	2.92	2.9

table 2		E_1 (eV)	E_2 (eV)
	Al(111)	0.86	0.24
	Al(100)	0.95	0.25
	Na(110)	0.71	0.20

4. References

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