CHAPTER VI

CONCLUSION

We mention in this chapter the general and interrelated result which has not been clearly discussed in the previous chapter.

All bulk properties, such as density of states, Fermi level, local density distribution of electron etc., are perturbed by the surface. The effect is very complicate. Therefore only 3-D SIC is used to study the effect of surface on the properties. Even with a very simple SIC model only limit of small surface perturbation having simple cubic lattice structure with (001) surface plane is considered. It has been shown that the phase shift is small. The phase shift tends to zero for the ideal unperturbed SIC. We first work with the ideal unperturbed SIC. The work is then extended to the slightly perturbed SIC. It is shown that the effect of the surface on density of states is very small, while the effect on a wave function is large. The result is then applied to calculate the dispersion part of the self-energy Σ_o. The result indicates the possibility of 3-D calculation of the chemisorption problem (in Newns-Anderson model). The absorption part of the self-energy is easily obtained by using Hilbert transformation. We can also calculate the other self-energy such as Σ_m, Σ_n etc. by changing the $(\omega - \epsilon_k)$ in F.1 to be $(\omega - (\epsilon_k + Um_\sigma))$, $(\omega + \epsilon_k - 2\epsilon_\ell - Un)$, etc., respectively.

Our 3-D results can be reduced to the 1-D limit. In this limit the wave function is exactly the same as that obtained by direct 1-D calculation, while the Σ_0 is exactly the same as the Newns' semi-elliptic form. Since our 3-D SIC has the simple cubic lattice structure with (001) surface plane, its 1-D limit corresponds to the linear chain of the same kind of atom. Alternately speaking, Newns' work is the limiting case of 3-D picture of ideal unperturbed SIC having simple cubic structure with (001) surface plane or of any SIC having all crystal layers have the same lattice structure as surface layer. As we know there are no transition metals having such lattice structure. To consider the 1-D limit which corresponds to 3-D lattice structure, we map out different types of layers in 3-D to correspond to different atoms in 1-D, e.g. FCC with (111) surface plane to be linear chain of

$$0, \quad 1', \quad 2'', \quad 3, \quad 4', \quad 5'', \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad .$$

To study the correlation effect, we start with Hubbard's two pole Green function. Then the HH, BH and BS are discussed in detail. We use Anderson Hamiltonian with different decoupling schemes to obtain HF, HH, BM and BS results. The matrix formalism is used to solve the single particle Green function. This method has the advantage of being simple short time and all single particle Green function being shown explicitly, except the BS scheme that the formalism can not be applicable. This is not the failure of the formalism for the reason that if we can find the matrix transformation that relates the two particle Green function to the single particle Green function, the problem is then solved. All the approximations discussed above clearly go beyond the HF and show the two poles in the Green function.

In contrast to BM. we have used the Anderson Hamiltonian since all parameters in the Hamiltonian can be treated semi-empirically. We find that BM decoupling scheme can be generalized. The generalized BM scheme can explain the domain that $m_\sigma \neq 0$ and $n \neq 1$, and also the magic number 2 in front of the self-energy Σ_o in the expression[98]

$$\Sigma_A = 2\Sigma_o - \Sigma_{n=1} \; .$$

The scheme also shows that the positive hole can play an interesting role. This is reasonable as we know that near the metal surface the electron density oscilates (Friedel osciliation)[7,65,66] and the impurity atom must be surrounded by positive hole (see chapter IV). The term $2\epsilon_\ell + Un$ in the pole of Σ_n shows something which is related to electronegativity ($X^M = (I + A)/2$). Unfortunatly, the detail interpretation needs deeper analysis.

The physical interpretation which is given to describe the correlation effect is given only as rough interpretation. Of course we know that the pole of any Green function can be interpreted as a quasi-particle.[88] However we can not always find their mass and other properties which can prove their existence. Thus future work will be the study of the existence of the two propagators as quasi-particle.

The development of chemisorption theory depends on development of the transition metals electronic structure, the surface phenomena and the impurity problem (localized magnetic moment in metals). Further development of chemisorption theory can occur when these three fields are further developed.