V.M.Burdeynyy

V.Kh.Kassiyanenko

TIGHT BINDING APPROXIMATON FOR ELECTRON SCATTERING BY PERIODIC STEP STRUCTURE ON ATOMIC SURFACE OF CRYSTAL

Vinnytsia national technical university

Анотація

Досліджується взаємодія електронів з віцинальною поверхнею, яка утворена терасоподібним періодичним розподілом атомів на граничній поверхні кристалу. Електронна система розглядається у наближенні сильного зв'язку, яке дозволяє врахувати збурення, внесене віцинальною поверхнею, безпосередньо в операторі Гамільтона.В однозонній версії наближення сильного зв'язку обчислено матричні елементи переходів, викликаних розсіянням електронів на терасах віцинальної поверхні. Показано, що ймовірність переходу містить інтерференційні компоненти і ефект перехресного розсіяння як на терасах, так і на стінках сходинок.

Ключові слова: *віцинальна поверхня, інтеграли перекриття. оператор збурення, амплітуда квантових переходів.*

Abstract

The interaction of electrons with the vicinal surface, which is formed by a terrace-like periodic distribution of atoms on the boundary surface of the crystal, is studied. The electronic system is considered in the tight-binding approximation, which allows to take explicitly into account the perturbation introduced by the vicinal surface directly in the Hamilton operator. It is shown that the transition probability contains interference components and the cross-scattering effect both on the terraces and on the walls of the steps.

Key words: *vicinal surface, overcup integrals. perturbation operator, amplitude of quantum transitions.*

In the process of crystal growth, its atomic surfaces formed by self-assembling technology, as a rule, are not atomically smooth purely atomic planes.Rally on the surface of growth the appearance of terraces and steps take place.Interacting by repulsive forces they push away from each other and finally usually create periodic structures known as vicinal surfaces. An example of such structures is illustrated in Fig.1
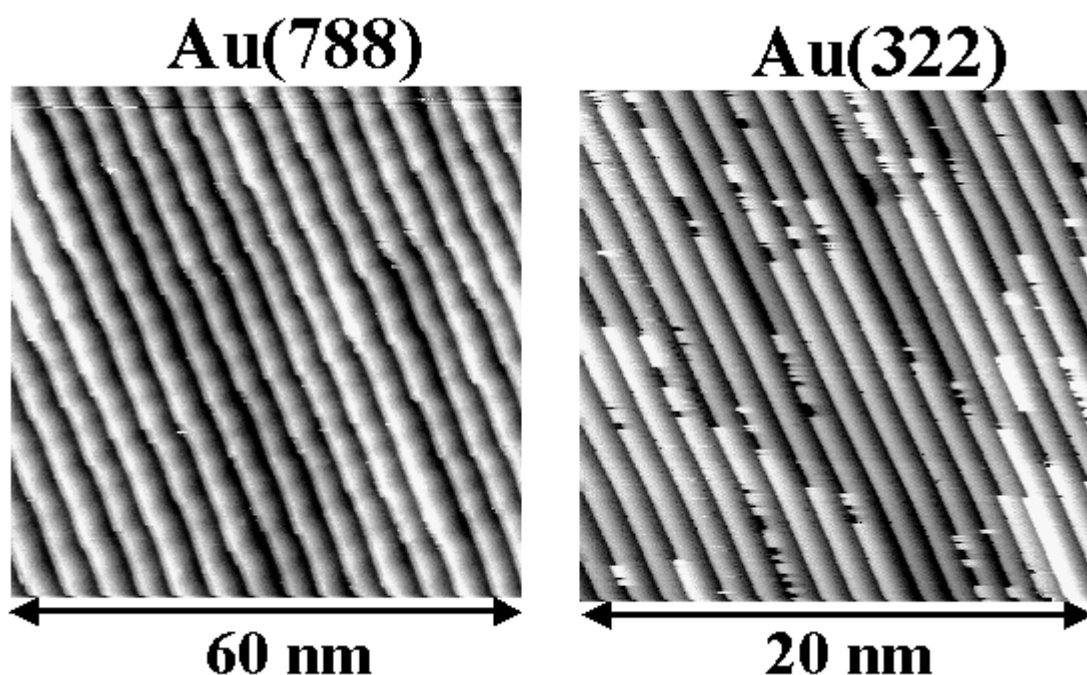
The study of electronic states on vicinal surfaces and the scattering of electrons by these surfaces manifests considerable practical interest. Referring to examples. represented in [1], it is worth to subline that the periodic system of terraces acts as a model structure for studying the one-dimensional and two-dimensional confinement of electrons and crossover between these types of electron capture and localization. As it turns out vicinal surfaces admit to be considered as ideal templates for creating self-assembled nanoobjects, such as quantum nanowires or ordered superstructures from quantum dots. Besided it once more importantn fact, that vicinal surfaces are associated with well promissing improvements of catalytic processes technology, has to be pointed out without of doubts.

As a rule, in theoretical studies of the electronic properties of periodic surface lattices, which are vicinal surfaces, the approximation of free electrons is basic and allows to explain majority of experimental results. . However, in some crystals, for example in transition metals, a considerable contribution to the electron density is determined by strongly localized d lectrons, for which the approximation of tight-binding electrons is more adequate. That is why the scattering of electrons by vicinal surface, which here is described by the approximation of tight-binding electrons, is an object of investigation in the terms of a simple model.

We consider a crystal with a simple cubic lattice with a period a in the approximation of a tight-binding electrons with the interaction between the nearest neighbors. Because of this feature of interaction the vicinal surface consisted of periodic repetition of terraces and steps, can be created by exclusions of interatomic bonds between atomic surfaces, which for the two-dimensional case is schematically shown in Fig.2
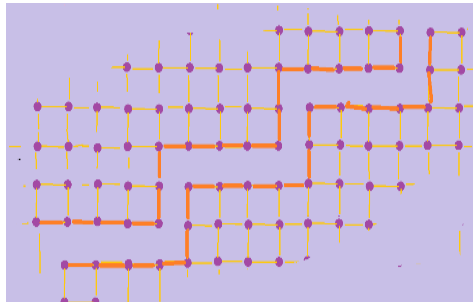

Fig.2 Two-dimensional illustration of the model of the vicinal surface

In Figure 2, the segments connecting the nearest atoms represent the chemical bonds described by the overlap integrals. By removing these connections, two unconnected broken lines are obtained. In the three-dimensional case they will correspond to a terrace-like surface lattice. The aim of the study is to calculate and analyze the probability of quantum transitions due to scattering of electrons by the vicinal surface with the width $l = sa$ of the terrace and the height $h = \gamma a$ of the step. It should be emphasized that the natural small parameter of the model is the angle of miscut, which is determined by the ralation $tg\alpha_m = \gamma / s$.:. Taking into account that the periodic step-like system in the approximation of the nearest neighbors is created by exlusion of chemical bonds between the nearest atoms belonging to the vicinal surfaces (as shown in Fig.2 there are two surfaces), for the secondary quantized perturbation operator determined in the node representation, follows the expression:

$$H_c = -W(a_y)\sum_{l,r}\sum_{n=p+rs+r+1}^{p+(s+1)(r+1)}\left[a^\dagger_{l,n,\bar{\alpha}+r(\gamma+1)}a_{l,n,\bar{\alpha}+r(\gamma+1)-1} + a^\dagger_{l,n,\bar{\alpha}+r(\gamma+1)-1}a_{l,n,\bar{\alpha}+r(\gamma+1)}\right] -$$

$$-W(a_x)\sum_{l,r}\sum_{\alpha=\bar{\alpha}+r(\gamma+1)}^{\bar{\alpha}+(r+1)(\gamma+1)}\left[a^\dagger_{l,p+r(s+1)+2,\alpha}a_{l,p+r(s+1)+1,\alpha} + a^\dagger_{l,p+r(s+1)+1,\alpha}a_{l,p+r(s+1)+2,\alpha}\right]$$

Here, the term in the first line is responsible for rupture of chemical bonds on the horizontal surface of the terrace, and the term belonging to thesecond provides their rupture on the vertical wall of terarace. In addition generally accepted notation of the operators of creation $a^{\dagger}_{l,n,\alpha}$ and aniquilation $a_{l,n,\alpha}$ of electrons in nodes with Cartesian coordinates (l,n,α) is applied.. The transition from the operators of creation я $a^{\dagger}_{l,n,\alpha}$ and aniquilation $a_{l,n,\alpha}$ at lattice nodes to the operators of creation and aniquilatiion of electrons in a state with a certain value of the wave vector is carried out according to the usual algorithm, namely:

$$a^{\dagger}_{l,n,\alpha} = \frac{1}{\sqrt{N_x N_y N_z}} \sum_{q,k,Q} a^{\dagger}_{q,k,Q} \exp\left[i(ql + kn + Q\alpha)\right]$$

$$a_{l,n,\alpha} = \frac{1}{\sqrt{N_x N_y N_z}} \sum_{q,k,Q} a_{q,k,Q} \exp\left[-i(ql + kn + Q\alpha)\right]$$

By substituting these decompositions over plane waves in the perturbation operator after calculating the sums over nodes of crystal lattice, the perturbated part of Hamiltonian operator $H_c(p,\bar{\alpha})$ turns out modified to the following form

$$H_c(p,\bar{\alpha}) = -\frac{\pi\xi}{2N_x N_y} \times \sum_{q,k,k',Q,Q'} \left\{ \delta[1 - Cos(\Delta k(s+1) + \Delta Q(\gamma+1)] \times \right.$$

$$\times \left[W(a_y)(e^{iQ'} + e^{-iQ})\exp\left(i\Delta k[p+1] + i\Delta Q\bar{\alpha}\right)\frac{(1 - e^{i\Delta k(s+1)})}{1 - e^{i\Delta k}} + \right.$$

$$\left. + W(a_x)(e^{ik} + e^{-ik'})\exp\left(i\Delta k[p+1] + i\Delta Q\bar{\alpha}\right)\frac{(1 - e^{i\Delta Q(\gamma+1)})}{1 - e^{i\Delta Q}} \right] a^{\dagger}_{q,k,Q} a_{q,k',Q'} \right\}$$

It is well known that the scattering of carriers or other elementary excitations is crucial for most of the effects that occur in condensed systems. The exchange of energy and momentum due to the transition to equilibrium or steady state is carried out through the collision of carriers with structural defects of various natures or elementary excitations, such as phonons, magnons, or other carriers. As the size decreases, the scattering role at the sample boundaries increases. This scattering mechanism becomes dominant for granular metals, metal clusters, semiconductor quantum dots when the characteristic grain size, clusters , quantum dots or terrace geometric parameters, as it takes place in this study ,become smaller than the average free path length due to the above mentioned mechanisms, ie there is a transition from relaxation to diffusion mode. . The scattering cross section is determined by the golden Fermi rule [3], which is based on the square of the modulus of the quantum transitions amplitudes, for which in the case of here proposed model of vicinal surface has been found the following final relationship:

$$\left| \langle k,Q | H_c(p,\bar{\alpha}) | k',Q' \rangle \right|^2 = \frac{2W^2(a)}{N^2} \left\{ [1 + Cos(Q + Q')]\frac{Sin^2 \Delta k(s+1)/2}{Sin^2 \Delta k/2} + \right.$$

$$\left. + [1 + Cos(k + k')]\frac{Sin^2 \Delta Q(\gamma+1)/2}{Sin^2 \Delta Q/2} + \right.$$

$$+4Cos\frac{Q+Q'}{2}Cos\frac{k+k'}{2}Cos[\Delta k(s-1/2)-\Delta Q(\gamma-1/2)]\times$$

$$\times\frac{Sin\Delta k(s+1)/2}{Sin\Delta k/2}\frac{Sin\Delta Q(\gamma+1)/2}{Sin\Delta Q/2}\Bigg\}\delta_{Cos\Phi,1}$$

where the phase factor is determined by the expression $\Phi=\Delta k(s+1)+\Delta Q(\gamma+1)$.

The above formula is our main result which determines the intensity of quantum transitions. It is clearly visible that three terms can be distinguished in the final formula. They have the following interpretation:

a) The first term describes the multi-wave interference of electron waves scattered by atoms belonging to terraces.

b) Accordingly - the second term - determines the result of the interference of electron waves that are scattered by the atoms that form the steps.

c) The most interesting and non-trivial is the last term. This term describes the effect of cross-scattering on one step and has no analogues in scattering on an ideal atomic plane.

As far as the Kronecker factor $\delta_{Cos\Phi,1}$, it takes into account the periodicity of the studied structure and correspods to the Wolf-Bregg's condition well known for crystal Physics.

REFERENCES

1.Ortega J.E.,J. Lobo-Checa, G. Peschel, S. Schirone,Z. M. Abd El-Fattah, M. Matena,F. Schiller, P. Borghetti, P. Gambardella, and A. Mugarza, Scattering of surface electrons by isolated steps versus periodic step arrays, DOI: 10.1103/PhysRevB.87.115425

2.Ashcroft, W.Neil, N.David Mermin, Solid State Physics,Holt, Rinehart and Winston,1976,v.1, 310

3.Ландау Л.Д., Е.М.Лифшиц , Квантовая механика, нерелятивистская теория, М.. Госфизматгиз, 1962,704.
.

Бурдейний Володимир Мефодійович,кандидат фізико-математичних наук,доцент, професор кафедри загальної фізики, Вінницький національний технічний університет, м.Вінниця. brdnvldmr@ukr.net

Касіяненко Василь Харитонович, доктор фізико-математичних наук, професор, завідувач кафедри загальної фізики, Вінницький національний технічний університет, м.Вінниця.

Burdeynyy Volodymyr Mefodiyovych, PhD in Physics and Mathematics, associated professor of General Physics Department, Vinnytsia National Technical University, Vinnytsia , brdnvldmr@ukr.net

Kassiyanenko Vasul Kharutonovuch, Doctor of Sciecies in Physics and Mathematics, professor, Chief of General Physics Department, Vinnytsia National Technical University, Vinnytsia .