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ИНСТИТУТА
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SURFACE RELAXATION IN α -IRON

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1. INTRODUCTION

Recently, experimental surface relaxation data have become available for α - from^{/1/}. The first attempt to explain these data within the framework of an empirical lattice model was published by Johnson^{/2/}.

At present, it is not clear whether interatomic potentials can be deduced from first principles in the case of transition metals^{/3/}. Some applications of empirical interaction model in b.c.c. transition metals indicate that the volume or angle dependent term (describing many-body interaction) + central two-body potential provide a satisfactory description of interaction in bulk crystals^{/4-8/} and lead also to a reasonable estimate of surface cleavage energies^{/9/}. However, more detailed studies of surface defects are still at an earlier stage of development. Since modelling of free surfaces is of a great significance in many problems, the aim of the present study is to investigate the possibility of applying an empirical many body interaction model in this field.

If one two-body (or many body) interatomic forces which obey the equilibrium condition in a bulk crystal (e.g.) the zero - stress conditions or including the non-zero initial stresses arising from the volume dependent term) then generally, there are unresolved forces at the surface which must be either compensated by external forces or relaxed to obtain a free surface. Note that in recent works^{/10-12/} concerning crack extension simulations, the external forces have been incorrectly used to compensate unresolved forces at the surface. In paper^{/2/}, an exponentially decreasing function of pressure containing two free adjustable parameters is supposed near the surface and the parameters are varied to obtain a reasonable agreement with experimental data for interplanar spacing near the surface. This model gives either zero displacements or compression near the surface. In the experiment however, also dilation was observed in some crystalline directions^{/1/}.

For some lattice defect simulations (such as crack extension), use of the same type interaction model is tempted in bulk and near the surface of a crystal. This paper looks at an application of an empirical lattice model from this point of view.

2. MODEL

2.1 Interatomic Interaction

Assuming that interaction between two atoms ℓ and ℓ' depends not only on their relative distance $r^2(\ell, \ell')$ but also on their local orientation in the lattice we may expand the potential function $\psi(r^2, \theta, \phi)$ in terms of spherical harmonics:

$$\psi(r^2, \theta, \phi) = \phi_0(r^2) + \sum_{m=1}^{+1} \phi_{1m}(r^2) Y_{1m}(\theta, \phi) + \dots + \sum_{m=-4}^{+4} \phi_{4m}(r^2) Y_{4m}(\theta, \phi) + \dots$$

The first terms, which satisfy cubic lattice symmetry requirements are

$$\psi(r^2, \theta, \phi) = \phi(r^2) + G(r^2) \{ Y_{4,-4} + Y_{4,4} + \sqrt{\frac{14}{5}} Y_{4,0} \} = \phi(r^2) + G(r^2) Y(\theta, \phi).$$

If we introduce unit vectors \vec{s}_1, \vec{s}_2 and \vec{s}_3 which represent the directions of main axes of the cubic crystal [100], [010] and [001], we can write for the angle dependent function

$$Y(\ell, \ell') = \frac{(\vec{s}_1 \cdot \vec{r}(\ell, \ell'))^4 + (\vec{s}_2 \cdot \vec{r}(\ell, \ell'))^4 + (\vec{s}_3 \cdot \vec{r}(\ell, \ell'))^4}{r^4(\ell, \ell')} - \frac{3}{5} \quad (2.1)$$

or

$$Y(\ell, \ell') = \frac{r_1^4(\ell, \ell') + r_2^4(\ell, \ell') + r_3^4(\ell, \ell')}{r^4(\ell, \ell')} - \frac{3}{5} \quad (2.2)$$

for a cartesian coordinate system parallel to the main cubic axes [100], [010] and [001]. Within the framework of this empirical model, the total energy per atom, equilibrium conditions and second order elastic constants in the bulk crystal take the form^{/7/}

$$E_1 = \frac{1}{2} \sum_{\ell}^{\ell \neq 0} \psi(\ell) = \frac{1}{2} \sum_{\ell}^{\ell \neq 0} \phi(\ell) + \frac{1}{2} \sum_{\ell}^{\ell \neq 0} G(\ell) Y(\ell), \quad (2.3)$$

$$S_{1m}^0 = \frac{1}{2\theta_0} \sum_{\ell}^{\ell \neq 0} \psi_1^0 r_m^0 = \frac{1}{2\theta_0} \sum_{\ell}^{\ell \neq 0} 2(\phi' + G'Y)_0 r_1^0 r_m^0 + G_1^0 Y_1^0 r_m^0, \quad (2.4)$$

$$C_{11} = [1111]^0, \quad C_{12} = [1212]^0, \quad C_{44} = \frac{1}{2} ([1122]^0 + [1212]^0), \quad (2.5a)$$

where

$$[ijmn]^0 = \sum_{\ell}^{\ell \neq 0} 4(\phi'' + G'' \cdot Y)_0 r_i^0 r_j^0 r_m^0 r_n^0 + G^0 \cdot Y_{ij}^0 r_m^0 r_n^0$$

and

$$\phi' = \left(\frac{\partial \phi}{\partial r^2} \right)_0, \quad G' = \left(\frac{\partial G}{\partial r^2} \right)_0, \quad \phi'' = \left(\frac{\partial^2 \phi}{\partial (r^2)^2} \right)_0, \quad G'' = \left(\frac{\partial^2 G}{\partial (r^2)^2} \right)_0,$$

$$Y_i^0 = \left(\frac{\partial Y}{\partial r_i} \right)_0, \quad Y_{ij}^0 = \left(\frac{\partial^2 Y}{\partial r_i \partial r_j} \right)_0.$$

Note that all quantities which enter the expressions denoted by subscript are related to the initial reference configuration without initial stresses - see eq. (2.4).

This empirical model leads to following three important consequences for a Bravais lattice with cubic symmetry:

- (i) $Y_i^0(\ell) = 0$ for all i and for each individual atom ℓ placed in the regular lattice position^{/7/}.
- (ii) The deviation from the Cauchy relations depends only on the non-central part $G(\ell) Y(\ell)$ of the potential:

$$C_{12} - C_{44} = 2P_c = \frac{1}{4\theta_0} \sum_{\ell} G^0(\ell) \{ Y_{12}^0(\ell) r_1^0(\ell) r_2^0(\ell) - Y_{11}^0(\ell) r_2^0(\ell) r_2^0(\ell) \}. \quad (2.5b)$$

- (iii) The contribution of the non spherical term to the total energy in reference configuration can be expressed by

$$E_y^0 = \frac{1}{2} \sum_{\ell}^{\ell \neq 0} G(\ell) Y(\ell) = + \frac{6}{5} P_c \theta_0, \quad (2.6)$$

where P_c is the Cauchy pressure given above. The relation (2.6) holds independently of the choice of the shape $G(r^2)$ and the range of interaction. The proof is given in Appendix. The relation (2.6) shows, that the nonspherical part $G(\ell) Y(\ell)$ of the potential represents a collective type of interaction in the lattice. Its contribution to the total energy of the crystal is positive for all b.c.c. transition metals since the value $C_{12} - C_{44}$ is positive for these metals.

Assuming a spherically distributed free electron gas, then energy density arising from kinetic energy of free electrons is^{/14/}

$$\omega^{\ell} = +A \left(\frac{\theta}{\theta_0} \right)^{-5/3}.$$

Neglecting other volume dependent terms, we can write for Cauchy pressure and for its contribution to the cohesive energy per atom the following relations:

$$2P_c = C_{12}^{\ell} - C_{44}^{\ell} = \frac{10}{9} A, \quad E^{\ell} = + \frac{9}{5} P_c \theta_0.$$

Of course, these values are too high because of neglecting the exchange and correlation effects in free electron gas. It follows from tight binding model that also d-band electrons contribute to the Cauchy pressure^{/9/}. The correct magnitude of these individual contributions is unknown for b.c.c transition me-

tals ^{/3/}. Nevertheless, it is clear that the exchange energy of free valence electrons ^{/13/} and the term arising from d-bands electrons ^{/3,9/} give a negative contribution to the energy, unlike the non-spherical part of our potential.

In connection with the above mentioned facts, the contribution $E_y^\circ = + \frac{6}{5} P_c \theta_0$ in our empirical model is possible to interpret as a contribution arising from the kinetic energy of non-spherically distributed valence electrons.

Point defect studies ^{/4-6/}, the estimates of the surface cleavage energies ^{/18/} and also surface relaxation data for α -Fe ^{/1/} indicate that except of the volume (density) or angle dependent terms, the short-range two body forces should be used for b.c.c. transition metals rather than long-range forces. Restricting the interaction to the first nearest I and to the second next nearest II neighbours in the b.c.c lattice, we can write

$$E_I^\circ = 4\psi_I^\circ + 3\psi_{II}^\circ, \quad (2.7)$$

$$S_{im}^\circ = \frac{4}{a} (\psi_I' + \psi_{II}') = 0, \quad (2.8)$$

$$C_{11} = 2a\psi_I'' + 8a\psi_{II}'' + \frac{2^6}{27} \frac{1}{\theta_0} G_I^\circ, \quad (2.9)$$

$$C_{12} = 2a\psi_I'' - \frac{2^5}{27} \frac{1}{\theta_0} G_I^\circ, \quad (2.10)$$

$$C_{44} = 2a\psi_I'' + \frac{2^4}{27} \frac{1}{\theta_0} G_I^\circ - \frac{2}{\theta_0} G_{II}^\circ. \quad (2.11)$$

Here, due to symmetry of the relations (2.3)-(2.6), the following notation can be used:

$$\psi = \phi + GY, \quad \psi' = \phi' + G'Y, \quad \psi'' = \phi'' + G''Y.$$

It may be seen that instead of the construction of two pair potentials $\phi(r^2)$ and $G(r^2)$ in (2.3)-(2.6) we can search one effective interatomic potential $\psi(r^2)$ and the two appropriate constants G_I° and G_{II}° obeying the relations (2.7)-(2.11). The interatomic forces and force constants related to the atoms (0, ℓ) are then given by relations:

$$\psi_{\alpha}(0, \ell) = \frac{\partial \psi(0, \ell)}{\partial r_{\alpha}} = 2\psi'(0, \ell)r_{\alpha}(0, \ell) + G^\circ(0, \ell)Y_{\alpha}(0, \ell), \quad (2.12)$$

$$\psi_{\alpha\beta}(0, \ell) = \frac{\partial^2 \psi(0, \ell)}{\partial r_{\alpha} \partial r_{\beta}} = 2\psi''(0, \ell)\delta_{\alpha\beta} + 4\psi'''(0, \ell)r_{\alpha}(0, \ell)r_{\beta}(0, \ell) + G^\circ(0, \ell)Y_{\alpha\beta}(0, \ell). \quad (2.13)$$

2.2. Interplanar Interaction

Our preliminary numerical calculations and also the results of other authors ^{/17/} show, that the use of a classical two body potential with one minimum leads to surface relaxation displacements of opposite sign than in experiment. Adding of a volume dependent ^{/17/} or angle dependent term (present) does not change the situation.

To understand the reasons, it is very helpful to perform the estimates of surface relaxation within the framework of the model of interplanar interactions. In this paper we restrict our interest to the three basic directions $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ of b.c.c. lattice. The estimates will be performed within the framework of a harmonic approximation. In such an approach we need to know only the first and the second derivatives of the interplanar potential.

We will use the following notation to distinguish the space and the interplanar interaction:

x - direction of relaxation, $x = x \langle 100 \rangle$, $x \langle 110 \rangle$, $x \langle 111 \rangle$

U_i - interplanar potential

$$V_i = \frac{\partial U_i}{\partial x_i} - \text{interplanar forces}$$

$$W_i = \frac{\partial^2 U_i}{\partial x_i^2} - \text{interplanar force constants}$$

where $i = 1, 2, 3, \dots$ denotes the interaction between the first, the second and the third nearest planes and $x_i = x_1, x_2, x_3, \dots$ denotes the corresponding interplanar spacing.

Due to the symmetry of the cubic lattice, the non-zero unresolved forces arise only toward the direction perpendicular to the surface in the case of the crystallographic directions $\langle 001 \rangle$, $\langle 110 \rangle$, $\langle 111 \rangle$. The forces in these directions can be transferred through pure longitudinal mode of vibration which corresponds to the uniaxial strain in the direction perpendicular to the surface. For this reason, the interplanar interaction can be simulated by linear chain illustrated in Fig.2. The range of interplanar interaction is given by the range of interatomic - (see Fig.1). That means, if we consider the interaction between the first neighbours I and the second neighbours II in the space lattice, then we must consider 2 interacting planes in the $\langle 001 \rangle$ direction, only 1 interacting plane in the $\langle 110 \rangle$ direction and 3 interacting planes in the $\langle 111 \rangle$ direction.

The correct transition from space interatomic to interplanar interaction must fulfill the equilibrium condition of mechanical stability in the reference unrelaxed equidistant configuration of the infinite chain.

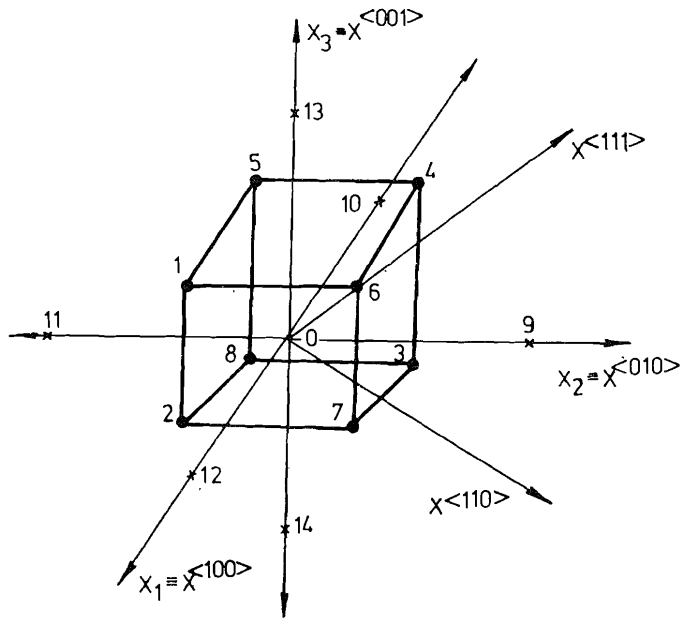


Fig.1. Short-ranged interaction in b.c.c. lattice.

If we consider homogeneous uniaxial deformation of a finite chain, then the change of energy is given by the relation

$$U^N - U_0^N = (N-1)V_1(d_0\epsilon) + (N-2)V_2(2d_0\epsilon) + (N-3)V_3(3d_0\epsilon) + \dots$$

$$+ \frac{1}{2}\{(N-1)W_1(d_0\epsilon)^2 + (N-2)W_2(2d_0\epsilon)^2 + (N-3)W_3(3d_0\epsilon)^2 + \dots\}.$$

The conditions of minimal energy in the underformed configurations are

$$\frac{\partial(U^N - U_0^N)}{\partial\epsilon} = 0, \quad \frac{\partial^2(U^N - U_0^N)}{\partial\epsilon^2} > 0, \quad \text{for } \epsilon = 0.$$

The first condition is fulfilled for a large N if

$$V_1 + 2V_2 + 3V_3 + \dots = 0. \quad (2.14)$$

The second condition is fulfilled for a large N if

$$\Delta U/N = \frac{1}{2}d_0^2\epsilon^2(W_1 + 4W_2 + 9W_3 + \dots) = \frac{1}{2}C_L^{\langle hkl \rangle}\epsilon^2\theta_0. \quad (2.15)$$

Here, d_0 denotes the equidistant interplanar spacing in the reference system for a given crystallographic direction $\langle hkl \rangle$, $C_L^{\langle hkl \rangle}$ is the elastic constant determining the velocity of longitudinal waves in this direction ($\rho\theta_L^2 = C_L^{\langle hkl \rangle}$) and $\Delta U/N$ is the strain energy per atom.

The individual interplanar potentials U_i , the forces V_i and the force constants W_i can be constructed by linear combinations of the correspondig interatomic quantities in a given direction:

$$V_i^{\alpha} = \sum_{\ell_1} a_{\alpha\beta} \psi_{\beta}(0, \ell_1),$$

$$W_i^{\alpha\alpha} = \sum_{\ell_1} a_{\alpha\beta} a_{\alpha\gamma} \psi_{\beta\gamma}(0, \ell_1), \quad (2.16)$$

where $a_{\alpha\beta}$ are directional cosines for the direction $X_{\alpha} = X^{\langle hkl \rangle}$. The direction $\langle 001 \rangle$ - see Fig.1,

$$U_1^{\langle 001 \rangle} = \sum_{\ell_1}^{1,4,5,8} \psi(0, \ell_1), \quad U_2^{\langle 001 \rangle} = \sum_{\ell_2}^{13} \psi(0, \ell_2), \quad U_3^{\langle 001 \rangle} = 0.$$

Equilibrium condition: $V_1^{\langle 001 \rangle} + 2V_2^{\langle 001 \rangle} = 0$.

Unresolved forces: if the free surface is placed to the point 0, - see Fig.1, then unresolved forces on individual planes 0, 1, 2, ..., per atom are given by the sum of missing interactions:

$$F_0^{\langle 001 \rangle} = F(0, 1') + F(0, 2') = V_1^{\langle 001 \rangle} + V_2^{\langle 001 \rangle},$$

$$F_1^{\langle 001 \rangle} = F(1, 1') = V_2^{\langle 001 \rangle}.$$

The direction $\langle 110 \rangle$

$$U_1^{\langle 110 \rangle} = \sum_{\ell_1}^{6,7,9,12} \psi(0, \ell), \quad U_2^{\langle 110 \rangle} = 0.$$

Equilibrium condition: $V_1^{\langle 110 \rangle} = 0$.

Unresolved forces: $F_0^{\langle 110 \rangle} = 0$.

The direction $\langle 111 \rangle$

$$U_1^{\langle 111 \rangle} = \sum_{\ell_1}^{1,4,7} \psi(0, \ell_1), \quad U_2^{\langle 111 \rangle} = \sum_{\ell_2}^{0,12,13} \psi(0, \ell_2),$$

$$U_3^{\langle 111 \rangle} = \sum_{\ell_3}^6 \psi(0, \ell_3), \quad U_4^{\langle 111 \rangle} = 0.$$

Equilibrium condition: $V_1^{\langle 111 \rangle} + 2V_2^{\langle 111 \rangle} + 3V_3^{\langle 111 \rangle} = 0$.

Unresolved forces:

$$F_0^{\langle 111 \rangle} = V_1^{\langle 111 \rangle} + V_2^{\langle 111 \rangle} + V_3^{\langle 111 \rangle},$$

$$F_1^{\langle 111 \rangle} = V_2^{\langle 111 \rangle} + V_3^{\langle 111 \rangle},$$

$$F_2^{\langle 111 \rangle} = V_3^{\langle 111 \rangle},$$

The interplanar forces and force constants can be determined from (2.16) taking the sum over the same atoms as for the corresponding interplanar potentials U_i .

2.3. Unified Description of Interatomic and Interplanar Interaction

The equations (2.8)-(2.11) concerning interatomic interactions and the forces and force constants for the interplanar interaction (2.16) can be re-written in a form more suitable for the construction of the empirical potential:

$$9G_{II}^{\circ} - 8G_I^{\circ} = 9\theta_0 (C_{12} - C_{44})/2 = 9P_c \theta_0, \quad (2.17)$$

$$\left(\frac{\partial\psi}{\partial r_I} \frac{2}{\sqrt{3}} + \frac{32}{9} \frac{1}{a} G_I^{\circ}\right) + \left(\frac{\partial\psi}{\partial r_{II}} - \frac{32}{9} \frac{1}{a} G_I^{\circ}\right) = 0, \quad (2.18)$$

$$\left(\frac{\partial^2\psi}{\partial r_I^2} - \frac{1}{a} \left(\frac{\partial\psi}{\partial r_I} \frac{2}{\sqrt{3}} + \frac{32}{9} \frac{1}{a} G_I^{\circ}\right)\right) = \frac{3}{2} a C_{12}, \quad (2.19)$$

$$\frac{\partial^2\psi}{\partial r_{II}^2} - \frac{1}{a} \left(\frac{\partial\psi}{\partial r_{II}} - \frac{32}{9} \frac{1}{a} G_I^{\circ}\right) = \frac{1}{2} a (C_{11} - C_{12}), \quad (2.20)$$

$$V_1^{<001>} = -2 \frac{\partial\psi}{\partial r_{II}}, \quad V_2^{<001>} = + \frac{\partial\psi}{\partial r_{II}}, \quad (2.21)$$

$$W_1^{<001>} = 2aC_{12} - \frac{4}{a} \left(\frac{\partial\psi}{\partial r_{II}} - \frac{32}{9} \frac{1}{a} G_I^{\circ}\right), \quad (2.22)$$

$$W_2^{<001>} = \frac{a}{2} (C_{11} - C_{12}) + \frac{1}{a} \left(\frac{\partial\psi}{\partial r_{II}} - \frac{32}{9} \frac{1}{a} G_I^{\circ}\right), \quad (2.23)$$

$$V_1^{<110>} = 0, \quad (2.24)$$

$$W_1^{<110>} = \frac{a}{2} (C_{11} + C_{12} + 2C_{44}). \quad (2.25)$$

$$V_1^{<111>} = -\frac{\sqrt{3}}{2} \frac{\partial\psi}{\partial r_{II}}, \quad V_2^{<111>} = \sqrt{3} \frac{\partial\psi}{\partial r_{II}}, \quad V_3^{<111>} = -\frac{\sqrt{3}}{2} \frac{\partial\psi}{\partial r_{II}} \quad (2.26)$$

$$W_1^{<111>} = \frac{a}{2} C_{12} - \frac{3}{a} \left(\frac{\partial\psi}{\partial r_{II}} - \frac{32}{9} \frac{1}{a} G_I^{\circ}\right), \quad (2.27)$$

$$W_2^{<111>} = \frac{a}{2} (C_{11} - C_{12}) - 2a(C_{12} - C_{44}) + \frac{3}{a} \left(\frac{\partial\psi}{\partial r_{II}} - \frac{32}{9} \frac{1}{a} G_I^{\circ}\right), \quad (2.28)$$

$$W_3^{<111>} = \frac{3}{2} a C_{12} - \frac{1}{a} \left(\frac{\partial\psi}{\partial r_{II}} - \frac{32}{9} \frac{1}{a} G_I^{\circ}\right). \quad (2.29)$$

Note that the dashed terms in (2.18) have been added only on the base of symmetry considerations.

From eq. (2.21) - (2.21) it follows that if the quantities $\left(\frac{\partial\psi}{\partial r_{II}}\right)_0$ and G_I° are chosen in such a way that they obey the sur-

face relaxation data, we may describe both surface effects and bulk properties (2.17)-(2.20) of the crystal by means of one effective potential

$$\psi_{\text{eff}} = \psi(r^2) + G_{\ell}^{\circ} Y(\theta_{\ell}, \phi_{\ell})$$

which has many body character through the angle dependent part $G_{\ell}^{\circ} Y_{\ell}$.

After relaxation the unresolved forces at the surface must vanish. Density change and the pressure S_{im} near the surface can be determined after relaxation from the new configuration positions $\{r_m\}$ of individual atoms and from the relation

$$S_{im}(\ell_k) = \frac{1}{2\theta_0} \sum_{\ell \neq \ell_k} 2\psi'(\ell_k, \ell) r_i(\ell_k, \ell) r_m(\ell_k, \ell) + G_{\ell}^{\circ} Y_{\ell}(\ell_k, \ell) r_m(\ell_k, \ell). \quad (2.30)$$

Here, $S_{im}(\ell_k)$ represents the pressure at the neighbourhood of the atom ℓ_k lying on the k -th plane near the surface. Because the relaxation displacements disappear very quickly^{/1,18/} with increasing distance from the surface, we can arrange both $S_{im}^{\circ} = 0$ near the surface.

3. RELAXATION

In this paper two procedures have been used to obtain surface relaxation data. The first procedure is based on the above mentioned model of linear chain and the second one on molecular dynamic simulations which have been performed on EC 1061 in JINR, Dubna.

3.1. Method of Linear Chain

The relaxed system of N plane $0, 1, 2, \dots, N-1$ modelled by linear chain - see Fig.2, will have a new configuration $x_0, x_1, x_2 \dots x_{N-1}$ which differs the original equidistant reference configuration in infinite crystal. The total potential energy $U^N(x_i)$ of the linear chain may be expanded in terms of displacement $\delta_i = x_i - x_i^{\circ}$.

Within the framework of harmonic approximation, the coefficients in Taylor series are just interplanar forces V_i and interplanar force constants W_i given above. From the requirements $\partial U^N / \partial x_i = 0$ which represent the condition of minimum $U^N(x_i)$ in the new configuration $\{x_i\}$, we obtain a system of N -linear al-

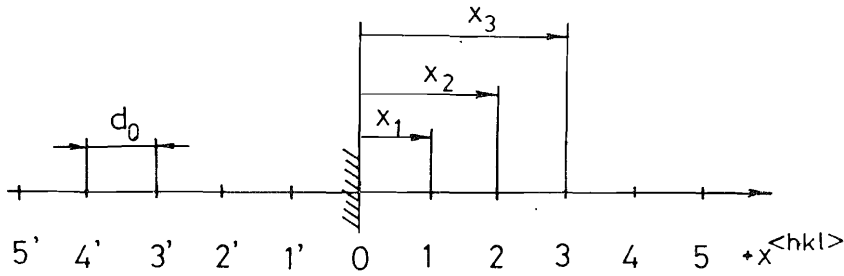


Fig.2. Model of linear chain.

gebraic equations for the displacement $\delta_0, \delta_1, \dots, \delta_{N-1}$ of individual plane. For a large N , the solution leads to the continued fraction. The solution procedure is described more precisely in ^{18/}. As a result it was found that the convergence of solution is very fast with respect to N . A reasonable estimate for the planar displacement can be obtained even for a small value of N .

Let us discuss the relaxation in the directions $\langle 001 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$.

The most simple case is the $\langle 110 \rangle$ direction. There are zero-unresolved forces on each individual plane and thus, all displacements are zero also.

The direction $\langle 001 \rangle$.

Taking $N=5$, it means the plane 0,1,2,3,4 in Fig.2, then it follows from symmetry considerations that $\delta_4 = -\delta_0$, $\delta_3 = -\delta_1$, $\delta_2 = 0$. The displacements δ_0, δ_1 can be evaluated from the system of equations

$$\begin{pmatrix} W_1 + W_2 & -W_1 \\ -W_1 & 2(W_1 + W_2) \end{pmatrix} \begin{pmatrix} \delta_0 \\ \delta_1 \end{pmatrix} = \begin{pmatrix} F_0 \\ F_1 \end{pmatrix} = \begin{pmatrix} -V_2 \\ +V_2 \end{pmatrix}. \quad (3.1)$$

The necessary conditions of stability in the new configuration is

$$V_2(\delta_1 - \delta_0) > 0, \quad (3.2)$$

where

$$\delta_1 - \delta_0 = V_2(W_1 + 3W_2) / \text{DET}. \quad (3.3)$$

It is obvious that the condition (3.2) can be fulfilled either if $V_2 > 0$ and $(\delta_1 - \delta_0) > 0$ or if $V_2 < 0$ and $(\delta_1 - \delta_0) < 0$. It follows from experiment ^{11/} that relative displacement $\delta_{10} = \delta_1 - \delta_0 = -0.02 \text{ \AA}$ for α -iron. That means, the requirement

$$\frac{\partial \psi}{\partial r_{II}} < 0 \quad (3.4)$$

concerning the potential $\psi(r^2)$ should be fulfilled.

The direction $\langle 111 \rangle$.

Taking $N=7$, it means the planes 0,1,2,3,4,5,6 in Fig.2, then $\delta_6 = -\delta_0$, $\delta_5 = -\delta_1$, $\delta_4 = -\delta_2$, $\delta_3 = 0$. The displacements δ_0, δ_1 and δ_2 can be evaluated from

$$\begin{pmatrix} W_1 + W_2 + W_3 & -W_1 & -W_2 \\ -W_1 & 2W_1 + W_2 & -W_1 + W_3 \\ -W_2 & -W_1 + W_3 & 2W_1 + 3W_2 + W_3 \end{pmatrix} \begin{pmatrix} \delta_0 \\ \delta_1 \\ \delta_2 \end{pmatrix} = \begin{pmatrix} F_0 \\ F_1 \\ F_2 \end{pmatrix} = \begin{pmatrix} V_1 + V_2 + V_3 \\ V_2 + V_3 \\ V_3 \end{pmatrix}$$

The relative displacements between the nearest plane are

$$\delta_1 - \delta_0 = \frac{\sqrt{3}}{2} \frac{\partial \psi}{\partial r} \{ (W_1 + 3W_2 + 2W_3)(W_2 + W_3) + W_2 W_3 \} / \text{DET}, \quad (3.5)$$

$$\delta_1 - \delta_2 = \frac{\sqrt{3}}{2} \frac{\partial \psi}{\partial r} \{ (W_1 + W_2 + W_3)(2W_1 + 4W_2 + 3W_3) - (W_1 + W_2) \} / \text{DET}, \quad (3.6)$$

the stability condition in the first approximation is

$$\delta_0(V_1 + V_2 + V_3) + \delta_1(V_2 + V_3) + \delta_2 V_3 > 0,$$

and it can be re-written as

$$\sqrt{3} \frac{\partial \psi}{\partial r_{II}} (\delta_1 - \delta_2) > 0. \quad (3.7)$$

The relative displacement $\delta_{10}^{\langle 111 \rangle}$ has been only determined in the experiment ^{11/} for the direction $\langle 111 \rangle$:

$$\delta_{10}^{\langle 111 \rangle} = (\delta_1 - \delta_0)^{\langle 111 \rangle} = -0.13 \text{ \AA} \text{ in } \alpha\text{-Fe}.$$

It follows from the relations (3.5), (3.6) and (3.7) that we may comply with both stability condition and experimental observation if the relation (3.4) is fulfilled.

3.2. Molecular Dynamic Simulations

In this method a cluster of M atoms with a given boundary conditions is considered. The atoms interact via a prescribed potential ψ . The problem is to integrate the equations of motion

$$m \ddot{\delta}_a(\ell) = \sum_{\ell'} \psi_a(\ell', \ell)$$

for each individual atom ℓ , starting from the initial conditions for displacements $\delta_a(\ell, t=0) = \delta_a(\ell)$ and for the velocities $\dot{\delta}_a(\ell, t=0) = \theta_a(\ell)$. Adding a damping term into the equations of motion

$$m \ddot{\delta}_a(\ell) + C \dot{\delta}_a(\ell) = \sum_{\ell'} \psi_a(\ell', \ell) \quad (3.8)$$

we may obtain static solution of the problem using a suitable

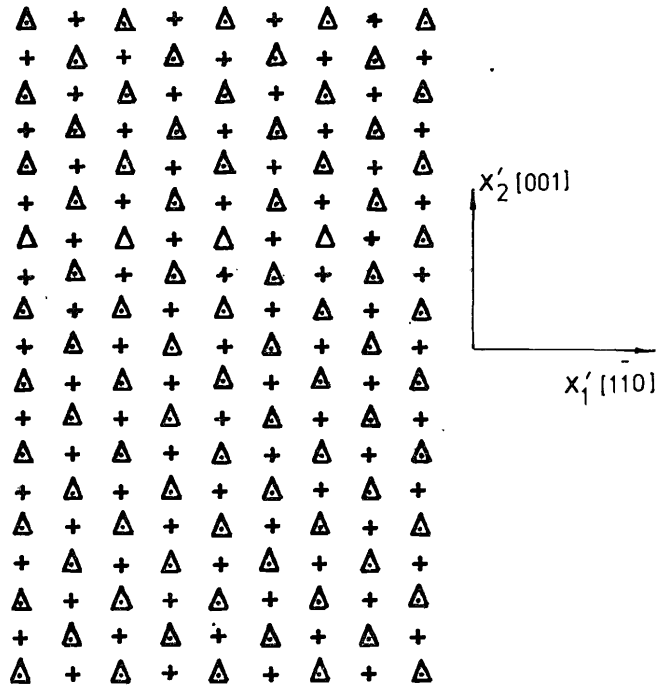


Fig. 3. Cluster for molecular dynamic simulations.

value of damping. (This is the so-called method of dynamical relaxation). In this paper central difference method is used for numerical integration and the damping term is chosen as

$$C = \alpha \mathbf{m}, \quad \alpha = 2\xi_r \omega_r,$$

where α is the damping coefficient, ξ_r weighting factor and ω_r the angular frequency of r -th mode vibration.

We have performed the numerical simulations of $\langle 001 \rangle$ surface relaxation in α -Fe with a cluster illustrated in Fig. 3. The atoms denoted by + lie in the plane (110), identical with the plane of paper. The atoms denoted by Δ represent in a fact two layer of atoms lying below and above the plane of paper. For example, it is the atom 5 and 6 in Fig. 1, projected on the plane (110). The boundaries in the directions $\langle 001 \rangle$ were free of external forces. At the boundaries $\langle 110 \rangle$ and $\langle \bar{1}\bar{1}0 \rangle$, the mirror forces have been applied to simulate an infinite dimensions in these directions.

The number N of the (001) plane in the cluster was changed and damping coefficient α has been chosen in dependence on this number. The time integration step $\Delta t = 0.1 \cdot 10^{13}$ sec was used in all presented calculations. The initial level of unresolved forces at the (001) surface was about 10^{-9} N. The model was consid-

ered to have converged when resultant force on individual atoms was about 10^{-12} N.

3.3. Numerical Results

We have performed the numerical calculations with three various interatomic potentials for α -Fe.

(A) Central pair potential $\psi = \phi(r) = (r-d)^2 (c_0 + c_1 r + c_2 r^2)$
 The parameters of the potential have following values: $a = 2.866 \text{ \AA}$
 $d = 1.35 a$, $c_0 = 0.4326586 \cdot 10^{22} \text{ J/m}^2$; $c_1 = -0.29155 \cdot 10^{12} \text{ J/m}^3$
 $c_2 = 0.4116859 \cdot 10^{21} \text{ J/m}^4$. They have been determined from the relations (2.8)-(2.10) taking $G_I^0 = G_{II}^0 = 0$ and $C_{11} = 2.43 \cdot 10^{11} \text{ N/m}^2$ and $C_{12} = 1.38 \cdot 10^{11} \text{ N/m}^2$. The dynamical relaxation has been performed for the following number of (001) plane:

- (i) $N = 5$. The value $\delta_{10} = (\delta_1 - \delta_0)_{\langle 001 \rangle} = +0.09 \text{ \AA}$ was obtained after 30ty time integration step (denoted by NSTEP in Fig. 5-7) using damping coefficient $\alpha_{\text{HIN}} = 0.609 \cdot 10^{14} \text{ sec}^{-1}$ for the first mode ω_1 of vibration. The potential energy of the cluster was in initial configuration $E_0 = -0.1675 \cdot 10^{-18} \text{ J}$ and in final relaxed configuration $E = -0.1680 \cdot 10^{-18} \text{ J}$.
- (ii) $N = 19$. The value $\delta_{10}^{\langle 001 \rangle} = +0.089 \text{ \AA}$ was obtained after about 60ty time integration step using $\alpha_{\text{MAX}} = 0.2436 \cdot 10^{15} \text{ sec}^{-1}$ for

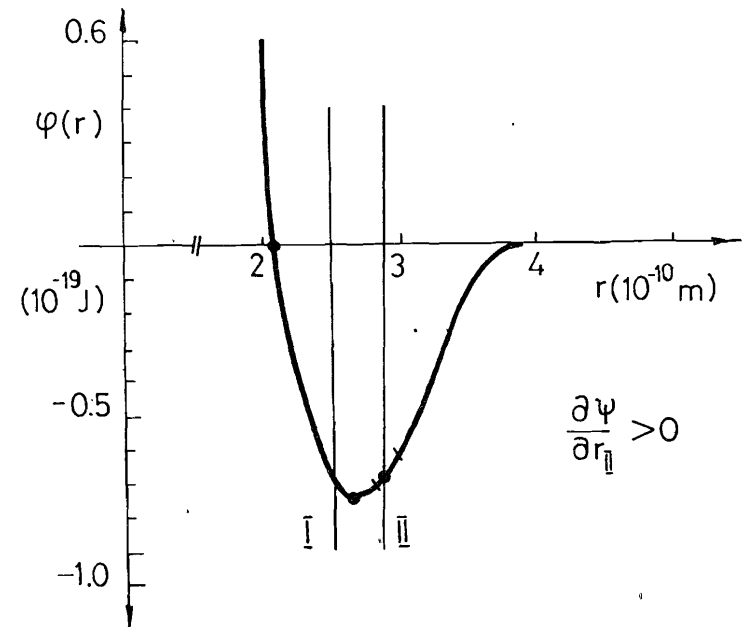


Fig. 4. Central pair potential $\psi(r) = (r-d)^2 (c_0 + c_1 r + c_2 r^2)$ for α -Fe.

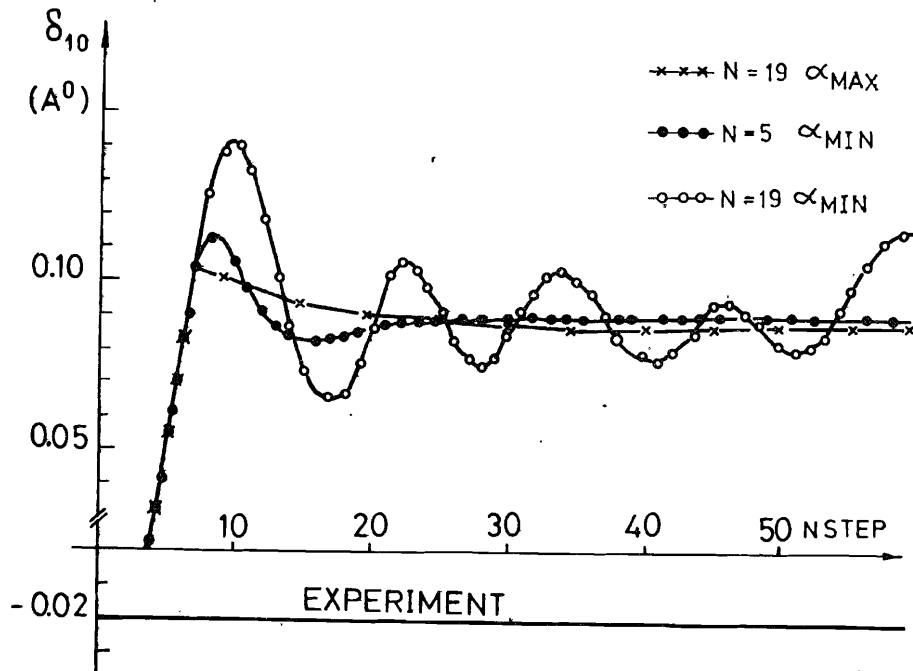


Fig. 5. Results of dynamical relaxation in the direction $\langle 001 \rangle$ with the potential $\phi(\mathbf{r})$ illustrated in Fig. 4.

the highest mode ω_{MAX} of vibration. The value $\alpha_{\text{MIN}} = 0.1354 \cdot 10^{10} \text{ sec}^{-1}$ before the lowest mode does not lead to the stationary solution - see Fig. 5. It may be seen that the convergence of solution with respect to N is very fast, the solutions for $N=5$ and $N=19$ lie close to each other. The potential energy has changed from $E_0 = -0.7377 \cdot 10^{-16}$ to $E = -0.7382 \cdot 10^{-16} \text{ J}$.

Comparison with the model of linear chain

If we evaluate the value $\partial\psi/\partial r_{\text{II}} = \partial\phi/\partial r_{\text{II}}$ for the central pair potential $\phi(\mathbf{r})$, the relative displacement δ_{10} in the direction $\langle 001 \rangle$ can be obtained from the equations (3.3) and (2.21-2.23): $\delta_{10}^{\langle 001 \rangle} = +0.088 \text{ \AA}$ for $N=5$. This estimate is in a very good agreement with the above given simulation results but does not agree with observed value $\delta_{10}^{\langle 001 \rangle} = -0.02 \text{ \AA}$. The reason is the positive value of $\partial\psi/\partial r_{\text{II}}$ for the used potential - see Fig. 4.

(B) Noncentral potential $\psi = \phi(\mathbf{r}) + G(\mathbf{r}) Y(\theta, \phi)$

Here $\phi(\mathbf{r})$ is the Morse potential $D\beta(\beta e^{-2\alpha r} - 2e^{-\alpha r})$ and $G(\mathbf{r}) = c(\mathbf{r} - \mathbf{r}_0) e^{-l/r_0}$. The parameters D, β, α and l, r_0 are given for α - Fe in /8/. This type of interatomic potential obeys all equations (2.7)-(2.11).

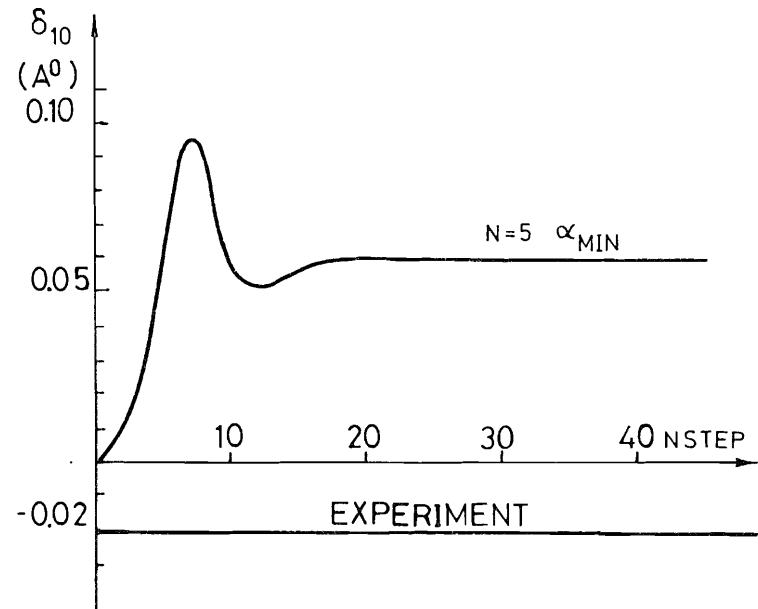


Fig. 6. Results of dynamical relaxation in the direction $\langle 001 \rangle$ with non-central potential $\psi(\mathbf{r}, \theta, \phi) = D\beta[\beta e^{-2\alpha r} - 2e^{-\alpha r}] + C(\mathbf{r} - \mathbf{r}_0) e^{-l/r_0} Y(\theta, \phi)$.

$N=5$. The value $\delta_{10}^{\langle 001 \rangle} = +0.06$ was obtained by the method of dynamic relaxation using $\alpha_{\text{MIN}} = 0.609 \cdot 10^{14} \text{ sec}^{-1}$ - see Fig. 6. For this potential, the second derivative $\partial^2\psi/\partial r_{\text{II}}^2$ is again positive - see /8/ and that is a reason of the discrepancy with experiment /1/. Thus, adding of non-spherical term does not improve the situation when it leads to a positive value $\partial\psi/\partial r_{\text{II}}$ of the total potential.

(c) Oscillating potential $\psi = \tilde{\phi}(\mathbf{r}) + G_0^0 Y(\theta_\ell, \phi_\ell)$

Here, the oscillating part of the potential has been taken as $\tilde{\phi}(\mathbf{r}) = c_4(\mathbf{r} - \mathbf{b})^4 - c_2(\mathbf{r} - \mathbf{b})^2 + c_0$. The parameters of the potential have been fitted using the equation (2.8) of zero initial pressure and using the equation for bulk modulus $B = (C_{11} + 2C_{12})/3$ which is obtained by linear combination of (2.9) and (2.10). The parameter \mathbf{b} was chosen nearly at the middle point between the first and the second neighbours in b.c.c. lattice. The numerical values of the parameters are: $c_4 = 0.1832 \cdot 10^{23} \text{ J/m}^4$, $c_2 = 0.2195 \cdot 10^2 \text{ J/m}^2$, $\mathbf{b} = 2.679 \text{ P \AA}$. The depth c_0 of the potential can be chosen either according to vacancy formation energy or according to surface cleavage energy. This value does not affect the relaxation - see eq. (2.17)-(2.29). With the above given potential, following calculations have been performed:

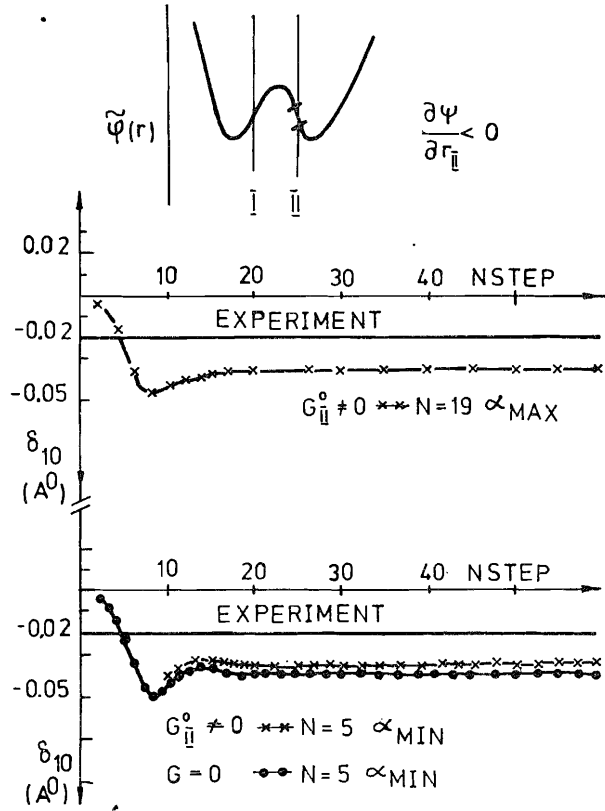


Fig.7. Results of dynamical relaxation in the direction $\langle 001 \rangle$ with oscillating potential $\phi(r) + G_{II}^0 Y(\theta_{II}, \phi_{II})$.

(i) $N=5$ and central part potential $\phi(r)$. The value $\delta_{10}^{\langle 001 \rangle} = -0.04 \text{ \AA}$ was obtained (see Fig.7) after relaxation using $\alpha_{\text{MIN}} = 0.0609 \cdot 10^{15} \text{ sec}^{-1}$. This value is twice higher but the same sign as the experimental value. The total potential energy of the cluster has changed from $E_0 = -0.13657 \cdot 10^{-17}$ to $E = -0.1375 \cdot 10^{-17} \text{ J}$ after relaxation.

(ii) $N=5$ and $\psi = \phi(r) + G_{II}^0 Y(\theta_{II}, \phi_{II})$, where the value of G^0 has been taken

as $G_I^0 = 0$, $G_{II}^0 = p \theta_0$. As may be seen from Fig.7, the value $\delta_{10}^{\langle 001 \rangle} = -0.0336 \text{ \AA}$ was obtained using $\alpha_{\text{MIN}} = 0.0609 \cdot 10^{15} \text{ sec}^{-1}$. The potential energy has changed from $E_0 = -0.7496 \cdot 10^{-18}$ to $E = -0.7593 \cdot 10^{-18} \text{ J}$.

(iii) $N=19$ and $\psi = \phi(r) + G_{II}^0 Y(\theta_{II}, \phi_{II})$, where $G_I^0 = 0$ and $G_{II}^0 = p_c \theta_0$. The value $\delta_{10}^{\langle 001 \rangle} = -0.0357 \text{ \AA}$ was obtained using damping coefficient $\alpha_{\text{MAX}} = 0.2436 \cdot 10^{15} \text{ sec}^{-1}$. The potential energy has changed from $E_0 = -0.4163 \cdot 10^{-17}$ to $E = -0.4173 \cdot 10^{-17} \text{ J}$.

4. CONCLUSIONS

The presented models of interatomic space interaction and interplanar interaction in the crystallographic directions $\langle 001 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ show that it is possible to describe successfully both bulk properties and surface relaxation data in α -iron if the second derivative of interatomic potential at the place of the second nearest neighbours in b.c.c. lattice is negative.

Three various types of interatomic potentials have been tested using non linear molecular dynamic simulations and the mo-

del of linear chain. The numerical results indicate that with oscillating potential obeying the condition $\partial\psi/\partial r_{II} < 0$, a reasonable agreement with the surface relaxation data in α -Fe can be achieved if an appropriate values of non-spherically term $G_{II}^0 Y(\theta_{II}, \phi_{II})$ are taken into account. The work will be continued in this field.

The author thanks Dr.V.K.Fedjanin, G.M.Gavrilenko, I.Mertig and N.M.Plakida for valuable discussions.

Appendix

The second derivatives Y_{ij} in eq.(2.5) are given^{7/} by the relation

$$Y_{ij} = -\frac{4}{r} \delta_{ij} \sum_k^{1,2,3} r_k^4 + \frac{24}{r} r_i r_j \sum_k^{1,2,3} r_k^4 - \frac{16}{r} r_i r_k^3 \delta_{jk} - \frac{16}{r^4} r_j r_k^3 \delta_{ik} + \frac{12}{r^4} r_k^2 \delta_{ik} \delta_{jk} \quad (A1)$$

Taking into account (A.1), (2.2) and performing partial summation over the first I, second II, third III, etc., neighbours in the lattice, the relations (2.5) and (2.3) turn out

$$(C_{12} - C_{44}) 2\theta_0 = \frac{1}{2} \{ G_I^0 \sum_{l_I} \frac{4r_2^2}{r^2} \left(\frac{r_1^4 + r_2^4 + r_3^4}{r^4} - \frac{3r_1^2}{r^2} \right) + \dots \} \quad (A2)$$

$$+ G_{II}^0 \sum_{l_{II}} \frac{4r_2^2}{r^2} \left(\frac{r_1^4 + r_2^4 + r_3^4}{r^4} - \frac{3r_1^2}{r^2} \right) + \dots \},$$

$$E_y^0 = \frac{1}{2} \{ G_I^0 \sum_{l_I} \left(\frac{r_1^4 + r_2^4 + r_3^4}{r^4} - \frac{3}{5} \right) + G_{II}^0 \sum_{l_{II}} \left(\frac{r_1^4 + r_2^4 + r_3^4}{r^4} - \frac{3}{5} \right) + \dots \} \quad (A3)$$

where $r \equiv r(\ell)$ and $r_i \equiv r_i(\ell)$ for $i = 1, 2$ and 3 . It is easy to verify that in every centrosymmetric cubic lattice the relation

$$\sum_{l_I} \left(\frac{r_1^4 + r_2^4 + r_3^4}{r^4} - \frac{3}{5} \right) = \frac{3}{10} \sum_{l_I} \frac{4r_2^2}{r^2} \left(\frac{r_1^4 + r_2^4 + r_3^4}{r^4} - \frac{3r_1^2}{r^2} \right) \quad (A4)$$

holds independently on the range of interaction $l_I = l_I, l_{II}, l_{III} \dots$. It is obvious from (A4) that (A3) can be written using (A2) as:

$$E_y^0 = \frac{1}{2} \sum_{\ell} G(\ell) Y(\ell) = \frac{3}{10} (C_{12} - C_{44}) 2\theta_0 = \frac{6}{5} p \theta_0$$

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Махова А.

E14-86-681

Поверхностная релаксация в α -железе

В работе предлагается эмпирическая модель взаимодействия в о.ц.к. решетке железа, которая позволяет описывать поверхностные явления и одновременно явления внутри кристалла. В случае железа α показано, что для согласия с экспериментальными данными по поверхностной релаксации необходимо применить эффективный потенциал взаимодействия, обладающий отрицательной производной в месте вторых ближайших соседей о.ц.к. решетки. Численные результаты были получены в рамках модели линейной цепочки и нелинейной молекулярной динамики.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна 1986

Machová A.

E14-86-681

Surface Relaxation in α -Iron

An empirical model of interaction in b.c.c. lattice is suggested. The model allows one to describe both surface effects and bulk properties of the crystal. It is shown that to obtain an agreement with surface relaxation data in α -Fe, the effective interatomic potential with a negative derivative at the place of the second nearest neighbours is required. Some numerical results have been obtained for α -Fe using the model of linear chain and non-linear molecular dynamic simulations.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Communication of the Joint Institute for Nuclear Research. Dubna 1986