ENERGY-BASED APPROACH TO LIMIT STATES IN NANOSTRUCTURES.
CALCULATION OF THE CRITICAL VALUES OF ENERGY FROM FIRST PRINCIPLES

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Summary The considered energy-based approach can appear helpful in the field of nanomechanics filling the gap between atomistic calculations and continuum mechanics modelling of the behaviour of different kinds of crystalline nanostructures. We propose to calculate the critical energy of pertinent proper states from quantum mechanical theory of nanostructures. The quantum mechanical model for an ideal single crystal of Cu is studied and the comparison with the results obtained for Al crystal is made.

Energy-based approach to limit states – the Rychlewski criterion

An energy-based approach to limit states in elastic solids of arbitrary anisotropy was developed by Rychlewski [1]. The Rychlewski limit condition is based on the theory of proper elastic states and the concept of energy orthogonal stress states, which make it possible to decompose additively the elastic energy density stored in an anisotropic body into not more than six disjoint parts. According to our opinion, the proposed approach can appear also helpful in the field of nanomechanics filling the gap between atomistic calculations and continuum mechanics modelling of the behaviour of different kinds of crystalline nanostructures [2, 3]. Under the limit state in nanostructures, we can understand the limit of linear elastic behaviour; although the other interpretations of the limit state are also possible. The energy-based criterion is formulated in terms of elastic strain states:

$$\frac{\lambda_1(\varepsilon_1)^2}{\Phi_1^{cr}} + \dots + \frac{\lambda_p(\varepsilon_p)^2}{\Phi_p^{cr}} \leq 1, \quad p \leq 6, \tag{1}$$

where $\lambda_1, \dots, \lambda_p$ are the Kelvin elastic moduli corresponding to the proper elastic states of the elastic stiffness tensor **S**, $\Phi_1^{cr}, \dots, \Phi_p^{cr}$ are the critical values of energy for each of the proper states, hence each term of the above criterion is the ratio of the accumulated elastic energy of the proper state to the critical one. The crucial point for the applications of the energy-based limit condition is to know the critical values of energy. They can be determined experimentally. However, it is difficult to measure it experimentally in the nano-scale. Therefore, we propose to calculate the critical energy of pertinent proper states from quantum mechanical theory of nanostructures. The analysis is confined to the cubic crystals. In such a case, three elastic proper states exist. They correspond to: a uniform expansion of a cube, equal contraction and elongation, respectively, along two cube edges, and change of the angle between the respective two edges of the cube.

The quantum mechanical model for Cu crystal

The quantum mechanical model for an ideal single crystal of Copper is studied. The assumed Born-Oppenheimer approximation enables the application of Bravais lattice to model the deformation of the crystal. Using the Wigner-Seitz cellular method, Fig.1, we replicate the radial density of the charge distribution calculated with the application of the Hatree method for a single Cu$^+$ ion, what results in the charge distribution for the crystal shown in Fig.2.
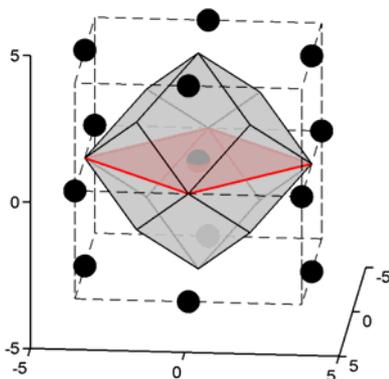

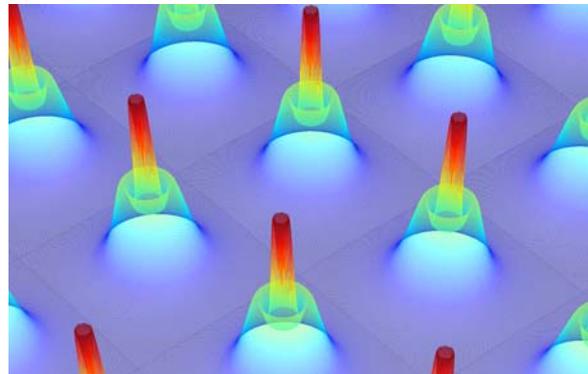Fig.1. Wigner-Seitz cell of Cu single crystal

Fig.2. The radial density of the charge distribution in the plane marked in Fig.1

Applying the calculated radial density of the charge distribution and using the Slater method [4], the structure of the *s, d, f* and *p* energy bands was calculated, Fig.3. The first qualitative analysis of the band structure was made by Krutter [5], whereas our numerical results make a basis for the calculations of the electron energy in deformed crystal. The energy bands are parameterised by the half distance "p" between the central ion and one of its nearest neighbours, cf. Fig.1. The parameter "p" is the controlling variable of the uniform extension of the crystal. The increase of the variable "p" produces

the gradual transition of the energy bands into the energy level. The particular interpretation has the transition of the energy band *s* into the energy level, which corresponds to the hypothetical disintegration of the crystal into the separate atoms, cf. Fig. 4.
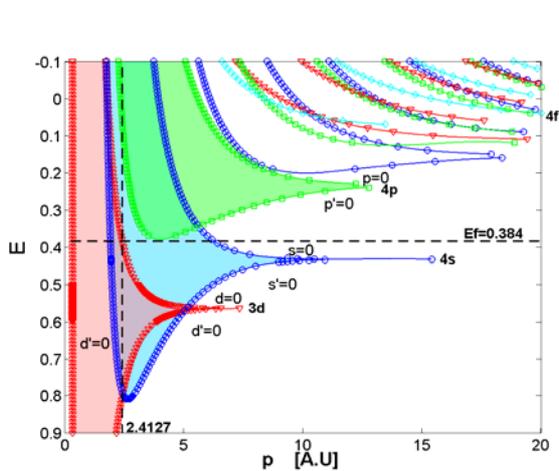

Fig.3. The calculated band structure of Cu crystal,
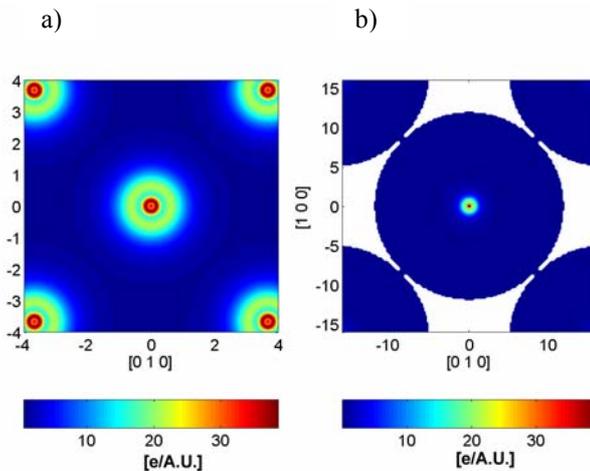p_{eq} = *2.4127* A.U.

a) b)

Fig.4. The calculated radial density of the charge distribution: a) in the equilibrium state, b) in the state of hypothetical disintegration of the crystal into the separate atoms.

The internal energy of the crystal volume $\Omega(p)$ confined in the expanding Wigner-Seitz cell was calculated from $(2)_1$, where the internal energy is the sum of the repulsive energy of the Cu^{11+} ions and the energy of the electrons of the energy bands *s* and *d*.

$$U(p) = U_{rep}(p) + \int_{-\infty}^{E_f(p)} E(p)\rho(E(p))dE(p), \qquad \Phi(p) = \frac{1}{\Omega(p)}\left[U(p) - U(p_{eq})\right], \qquad \Phi_1^{cr} = \Phi(p_{cr}). \qquad (2)$$
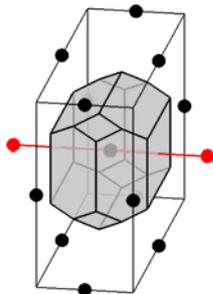

Fig.5. The Wigner-Seitz cell deformed according to the second proper state.

The similar analysis can be made for the deformation of the Wigner-Seitz cell according to the second proper state illustrated in Fig. 5. In such a case, the distance between the central ion and the neighbouring ones, marked in red, diminishes. This requires taking into account in the calculation of energy band structure the ellipsoidal charge distribution. The structure of the equations (2) leading to the calculation of the critical energy Φ_2^{cr} remains the same. For the third proper state, related with the change of the angle between the respective two edges of the cube, the similar algorithm of the calculation of the critical energy Φ_3^{cr} holds.

Conclusions

The similar identification of the energy-based Rychlewski criterion can be made for other crystals. The Al crystal was studied for the comparison. It posses the same symmetry as Cu, but has the different electronic structure, as for Al belongs to *sp*-valent metals. Therefore, the three critical energies are calculated, but by using the approximation of Nearly Free Electrons (cf. e.g. [6]). If we consider the relations between the critical energies, we can observe that it is the electronic structure that plays the crucial role in the strength distribution in the crystal of the same symmetry.

Literature

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