LATTICE DISTORTION MODEL. MODELING OF ELASTIC CONSTANTS ON CRYSTALLINE MATERIALS OF BCC-LATTICES

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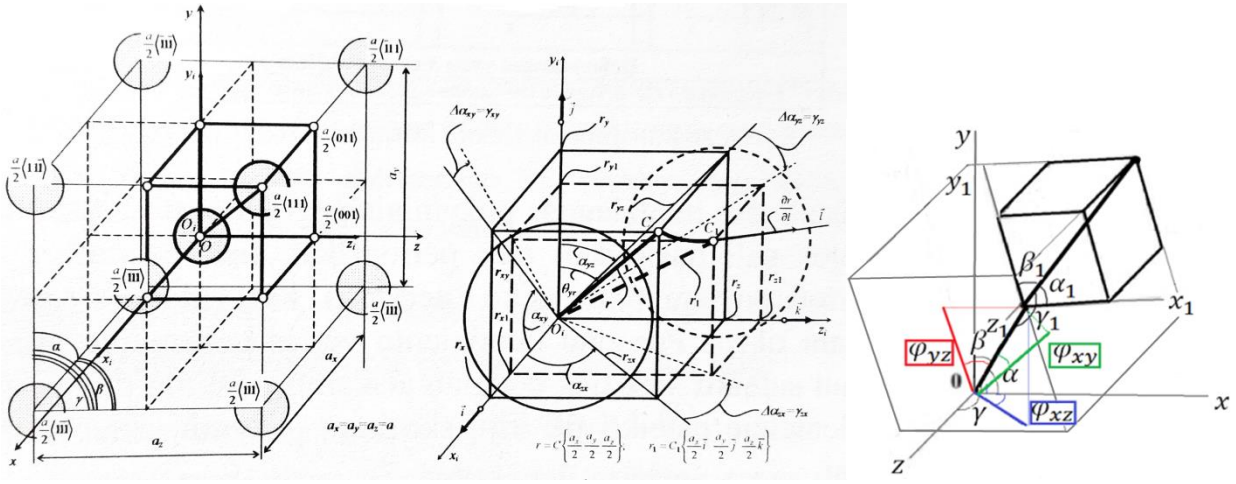
As the standpoint of this study is a creation of method based on the multi-scale modelling that was chosen as a way to collect and, in the case of high probability comparable with the experimental results or methods, to share all possible natural phenomena as some evidence of physical reality in crystalline materials. This method describes the complex behavior of atomic systems aligned by different spatial angles in neighbor microstructures. Virtually this allows us analyzing wave properties in discrete lattice/microstructure as the result of complex multi-directional neighbor impact. Firstly, the modeling of BBC-lattice deformation is presented according to the theory on computation of elastic constant like Poisson's ratio from the atomic perspective in close connection with experiment data obtained at macro-scale (Fig. 1). Poisson's ratio is expressed as:

$$\nu_i = -\frac{\varepsilon_{yi}}{\varepsilon_{xi}}; \qquad (1)$$

where $\varepsilon_{xi}(d_{xi}, \alpha_{xi}, C)$ and $\varepsilon_{yi}(d_{yi}, \alpha_{yi})$ – longitudinal and transverse deformation, C – coefficient of deformation intensity $1/\xi \le C \le 1/\xi^2$ while ξ - parameter which show one atom inertia to another according to the movement direction and depends on deformation level ($0 < \xi \le 1$).



(A) (B) (C)

Fig. 1. Lattice distortion model. A is BCC-lattice. The one eight of the lattice is taken in order to model relation between the nearest neighbor atoms in system Center-Edge. Axes XYZ represent the global coordinate system according to direction of impact. **B** is geometrical representation on physical model of lattice deformation in the local spatial coordinate system $X_1Y_1Z_1$. An edge atom draws path CC_1 explaining the spatial change in atomic distance and volume. **C** is the aligned BBC-lattice in both global and local coordinate systems. The angles α, β, γ are used in equations of tangent plane going at any single point of the outside surface of the unit sphere and for an evaluation of Burger's vectors <XYZ> [1]

Parallel to development in statistical mechanics, atomistic modeling is shown as a maturing and perspective tool in solid state physics and materials science and for the fine investigations of bulk characteristics and their elastic limits in crystalline materials.

[1] D. Raabe, M. Sachtleber, Z. Zhao, F. Roters, S. Zaefferer, Micromechanical and macromechanical effects in grain scale polycrystal plasticity experimentation and simulation Acta Materialia 17, pp. 3433-3441 (2001)