LATTICE DISTORTION MODEL ANALYSIS SIMULATING POISSON'S RATIO ON CRYSTALLINE MATERIALS OF BCC-LATTICES

Tomas Vaitkūnas[1], Audrius Jutas[1*]

[1] Department of Mechanical Engineering and Design, Kaunas University of Technology, Lithuania
tomas.vaitkunas@ktu.edu

We offered a lattice distortion model [1] which describes the complex behavior of atomic systems aligned by different spatial angles in neighbor microstructures. Poisson's ratio value of crystalline material ν_{sim} can be simulated without doing any experiment and expressed as average value of all groups' of materials lattices oriented at different angles interacting together during *l* number of peaks:

$$\nu_{sim} = \frac{1}{l}\left(\frac{1}{l}\sum_{k=1}^{l}\nu_{\max k} + \frac{1}{l-1}\sum_{k=2}^{l}\nu_{\max k} + \ldots + \nu_{\max l}\right); \quad (1)$$

where $\nu = \frac{1}{N}\sum_{i=1}^{N}\sum_{j=1}^{n}\frac{\nu_j}{n}$ is Poisson's ratio values of *n* lattices' groups interacting together, $\nu_j = -\frac{\varepsilon_{yj}}{\varepsilon_{xj}}$ is Poisson's ratio values of *j* group of lattices in the model, N is number of interactions in model, $\varepsilon_{xj}\left(d_{xj}, \alpha_{xj}, C\right)$ and $\varepsilon_{yj}\left(d_{yj}, \alpha_{yj}\right)$ is longitudinal and transverse deformation, C is coefficient of deformation intensity $1/\xi \le C \le 1/\xi^2$ while ξ is parameter which shows an intensity of one atom inertia to another according to the movement direction and depends on deformation level $(0 < \xi \le 1)$.

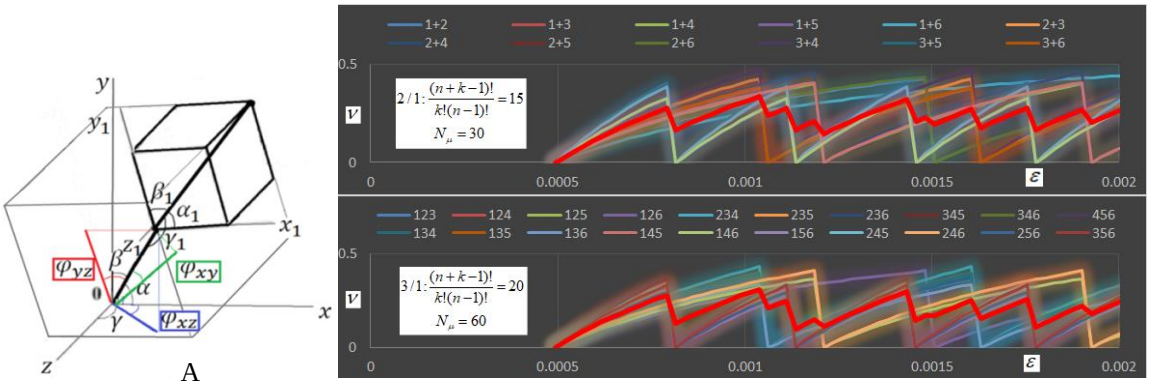

Fig. 1. Crystalline materials lattice distortion model: principles and stability. A is the aligned BBC-lattice in both global and local coordinate systems. The angles α, β, γ are used in equations of tangent plane going at any single point of the outside surface of the unit sphere and for an evaluation of Burger's vectors <XYZ> [2]. **B** shows simulated Poisson's ratio values of Iron when two groups of lattices interacting together (*n* = 2). In **C** Poisson's ratio values of Iron when three groups of lattices interacting together (*n* = 3) are given. Differences between results given in **B** and **C** pictures are not greater than 3 %. This fact confirms high model stability with different lattices interaction mechanisms.

Some corrections of this model can be done by evaluating the electron sublayers configuration in the lattice:

$$\nu = \nu_{sim} \cdot \left(1 + f_1\left(\sum x / \sum Y\right)\right); \quad (2)$$

where ν_{sim} is simulated Poisson's ratio value according to the equation (1), f_1 is weight function, $\sum x$ is sum of electrons in atom sublayers by their filling and $\sum Y$ is sum of electrons in the sublayer to be filled.

The model improvement from the perspective of sublayer filling by electrons increased proximity of simulated Poisson's ratio values to experimental by 53 %. In present study, the multiparametric atomistic model of crystalline materials is shown as a maturing and perspective tool in solid state physics and materials science. It can be used for the fine investigations of atomic states descriptive elastic characteristics of solid and comprehensive transformational evolution between differently aligned atomic systems and neighbor grains of microstructure. For the quantitative analysis, further studies are directed to creation of exact models for other crystalline materials having BCC-lattice.

[1] Vaitkūnas, T, and Jutas, A. "Lattice Distortion Model and Probabilistic Analysis Simulating Elastic Behavior of Crystalline Materials" 16th International Conference of Young Scientists on Energy Issues, (CYSENI 2019), 23-24 May 2019, Kaunas, Lithuania (2019): 390-98. Web.

[2] 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)