MS49-P2 **Crystallographic orientations and mechanical properties of metals.** V.I. Slavov. *Cherepovets state university, Cherepovets, Russia.*
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Petch-Holl dependence $\sigma_T = \sigma_o^{-\frac{1}{2}}$ was establish in the middle of last century. Value "k" characterize a grain boundaries ability to pass deformation from grain to grain. However, in materials with small dimesions of grains, various grains or the different phases investigators have to do with not equilibrium structure for which value "k" is not constant. Exit a lot modern studies what show about violation Petch-Holl law and it often is not carry out exactly. Chemical composition, dislocation and fine structure, texture and the grain dimension, which exert influence on the mechanical properties of polycrystals.

In the present paper have shown a new sight on the grain crystallographic orientations role in polycrystals and their influence on the mechanical properties. The main topic presented paper is a theoretical approach to crystal orientation on the basis Crystallographic Indexes Periodical System (PSCI). Crystallographic indexes may be represented in form PSCI, which consist from eight groups (G) by accordance to with square indexes sum distribution. All components of axial or planar crystallographic orientations are subdivided on the seven types (N) with different lattice direction or different lattice planes (HKL) of unit cell relatively the main external internal axes of the sample. Any crystallographic orientations can be expressed across orientation symmetry groups (GSO) as four numbers ($NG_1G_2G_3$) in the three-dimensional space. Quantity of crystal GSO with a different unit cell equally 230 and exactly coincidient with 230 well-know space groups crystals.

Physical sense of crystallographic orientations in the polycrystalline consist in the resulting symmetry them interaction with stress field. Stress field with point of view symmetry limited only 14 second-order tensor groups. On the basis superposition principle crystals and stress field appear now perhaps for study three-dimension texture and it influence on mechanical properties of different materials.

For example were carry out investigation three-dimensional orientations in tube steel samples with different mechanical properties: σ_T = 439 MPa, σ_B = 557 MPa, δ_{10} = 27%, $KCV_{-50} = 218 - 245 \frac{J}{cm^2}$, B 7 95%, and σ_T = 466 MPa, σ_B = 579 MPa, δ_{10} = 25%

Keyword: crystallography.

MS49-P3 **The ARP/wARP model building suite and the Arpnavigator user interface.** Tim Wiegels,[a] Saul Hazledine, Victor Lamzin, [a]*EMBL Hamburg, Germany*
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ARP/wARP is a software suite for automated model building and refinement in macromolecular crystallography. The package is able to build protein, RNA/DNA, secondary structure, solvent and ligands into electron density maps. Version 7.3 of ARP/wARP has recently been released. This new version of ARP/wARP is able to identify common ligands from a specified blob of electron density. Algorithms that fit ligands to electron density have also been strengthened so that they are increasingly independent of the input and now screen all possible ligand conformations. ARP/wARP is distributed with a 3D graphics interface, Arpnavigator, that has been tailored to give visual feedback during model building. It is hoped that the interface provides a convenient way of building a macromolecular model, can be educational for novice users and is a useful tool for experts when solving model building problems. In release 7.3, the Arpnavigator user interface has been enhanced to give a clearer realtime view of the ARP/wARP model building algorithms and supports new file formats so that it fits easier into the workflows of researchers performing drug discovery. Here, we present an overview of the improved model building in ARP/wARP, show the interaction between Arpnavigator and model building and also introduce new functionalities.

Keywords: model building; refinement; software