S. S. GUSKOV, *E. V. CHUPRUNOV*. ON THE GEOMETRICAL ASPECT OF INFLUENCE OF ATOMIC STRUCTURE ON SHAPE OF MONOCRYSTALS

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The problem of dependence of the shape of crystals upon their atomic structure is considered. A new computational method of calculation of crystal is proposed. The atomic structure of a crystal is considered as a packing of hard spheres. The crystal face is represented as a cross-section of a crystalline fragment. Orientation of the face is determined by the Miller indic (*hkl*). The sum over the cross-section of the hard spheres is calculated per unit oarea and is denoted as *P*. It is necessary to shift the cross-section plane in the range of the interplanar d_{hkl} spacing. Maximum of *P* can be defined as a filling coefficient *Q*. The calculation of the coefficient *Q* allows to determine the largest faces of the shape of a crystal. The quantitative matching settlement shape with substantially apparent shape of synthetic compounds and minerals is conducted. The offered procedure is compared to the reference Bravais approach, based on calculation of a reticular density of facets. The medial hit rate settlement and real faces on sampling from 70 structures has constituted 0.66 ± 0.08 for the Bravais law and 0.85 ± 0.05 for the proposed procedure at the confidence coefficient 0.95.