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Theoretical modeling of zircon's crystal morphology according to data of atomistic calculations

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Zircon is an essential mineral that is used in the U-Pb dating. Moreover, zircon is highly resistant to radioactive exposure. It is of great interest in solving both fundamental and applied problems associated with the isolation of high-level radioactive waste. There is significant progress in forecasting of the most energetically favorable crystal structures at the present time. Unfortunately, the theoretical forecast of crystal morphology at high technological level is under-explored nowadays, though the estimation of crystal equilibrium habit is extremely important in studying the physical and chemical properties of new materials.
For the first time, the thesis about relation of the equilibrium shape of a crystal with its crystal structure was put forward in the works by O.Brave. According to it, the idealized habit is determined in the simplest case by a correspondence with the reticular densities Rhkl of individual faces. This approach, along with all subsequent corrections, does not take into account the nature of atoms and the specific features of the chemical bond in crystals. The atomistic calculations of crystal surfaces are commonly performed using the energetic characteristics of faces, namely, the surface energy (Esurf), which is a measure of the thermodynamic stability of the crystal face. The stable crystal faces are characterized by small positive values of Esurf.
As we know from our previous research (Gromalova et al.,2015) one of the constitutive factors affecting the value of the surface energy in calculations is a choice of potentials model. In this regard, we studied several sets of parameters of atomistic interatomic potentials optimized previously. As the first test model («Zircon 1») were used sets of interatomic potentials of interaction Zr-O, Si-O and O-O in the form of Buckingham potentials. To improve playback properties of zircon additionally used Morse potential for a couple of Zr-Si, as well as the three-particle angular harmonic potential. The other sets of interatomic potentials («Zircon 2, Zircon 3») differed from the first in that parameters was found with the help of quantum-chemical calculations of the structure «ab initio».The surface energies for different faces of zircon were calculated using Metadise code (Watson et al., 1996) at P4-3000 personal computer with Windows XP operating system. The computation time for one simple form was from 30 minutes to 12 hours. Calculations have shown that depending on the chosen model the surface energy of zircons faces several changes. For example, Esurf of face (331) obtained using models of potentials «Zircon 2», «Zircon 3» sufficiently similar (2.82 and 3.01 J/mol2 respectively). Meaning of Esurf of this face, calculated on the basis of set «Zircon 1» significantly lower (1,54 J/mol2). With regard to the face (100), it has low surface energies when selecting all three models, with a minimum value (1,14 J/mol2) in the model «Zircon 1».

References:
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