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Short-range order analyses of the amorphous-crystalline silicates using graph theory

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The structural analyses of atoms arrangement in the area of short-range order in the mechanically activated minerals of the Arctic zone: pseudowollastonite (α-CaSiO3) and titanite (CaTiSiO5) was provided from two approaches: WAXD and computer simulation. Method based on invariants of a graph was used for analyses of computer experiment results.
Amorphous pseudowollastonite was obtained by mechanical activation of the samples in a centrifugal planetary mill AGO-2 for 30 min in air. The mechanical activation of the titanite was carried out in centrifugal mills with different centrifugal factors: with 40 g for 30 min in air and in CO2 (ICTREMRM, Apatites) and with 95 g for 30 min, 13.5 and 19.5 hours in air (Petrozavodsk State University).
The X-ray diffraction patterns were registered in CuKα and MoKα radiation. The theoretical X-ray patterns of atom's configurations were calculated using the modified Debye's formula.
The result of pseudowollastonite grinding was a chemical reaction which led to the formation of calcium carbonate and silica. In general the chemical composition in regions of the short-range ordering corresponds to the formula CaSi0.997C0.014O3.02. Theoretically calculated distribution of scattering intensity for a model of mechanical mixture corresponded to the following ratio: 0.75 scattering intensity of the cluster consisting of four unit cells of pseudowollastonite disordered in a molecular dynamic (MD) experiment; 0.25 scattering intensity of the cluster consisting of one unit cell of CaCO3; 0.25 scattering intensity of the cluster consisting of one unit cell of α-SiO2. Characteristics of the arrangement of tetrahedra in main cluster (initial and disordered) were calculated using the method based on graph theory [1]. It was found that rings of three tetrahedra were broken as the result of molecular dynamics experiments and about 30% of tetrahedra were linked in a continuous chain. Besides, there were chains consisting from 2 to 8 tetrahedra in this configuration.
The structure of mechanical activated for 30 min titanite (centrifugal factor 40 g) satisfactorily described by the model of randomly disoriented clusters with the linear size 21;26;46 Å, which are constructed by translation along the crystallographic axes X,Y,Z and disordered as a result MD experiment.
Grinding of titanite in the mill with centrifugal factor 95 g in the same time leads to the formation of mechanical mixture of nanosized clusters of two types: 7;9;12 Å and 35;35;66 Å. Correlations in the arrangement of layers in the cluster were not observed. The size of the clusters is reduced to 7×9×7 Å and 21;15;13 Å after increasing the time of grinding to 13.5 h in the mill with a centrifugal factor 95 g. The disorder in the arrangement of atoms was increased.

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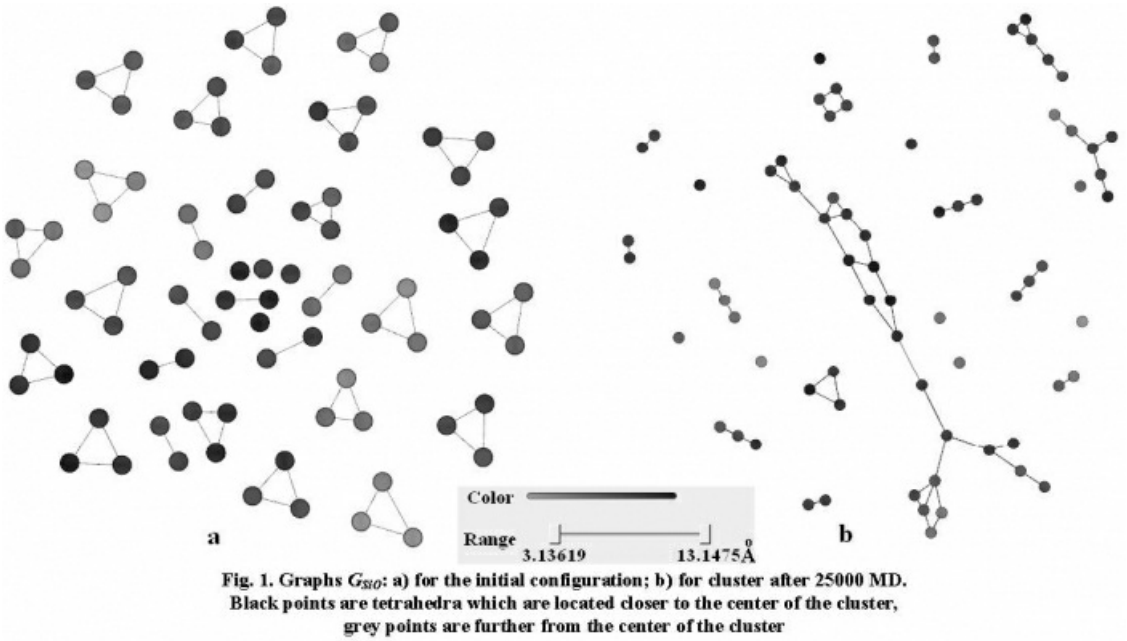

Fig. 1. Graphs G_{SiO}: a) for the initial configuration; b) for cluster after 25000 MD. Black points are tetrahedra which are located closer to the center of the cluster, grey points are further from the center of the cluster

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