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ABSTRACTS



we observed the increase of differentiation along this soil profiles. The content of Si in alkaline extract was changed in the same fashion that in the sour solution.

Summing up we can conclude that intensive agriculture destroys the silicon state and balance in ecosystem by means of plants (out irretrievable with crop). The transformation of silicon compounds in upper soil horizon results in degradation as living part of ecosystem as mineral part and general destruction of land. Because of this it is necessary to restore silicon state and balance in agro-ecosystems.

We have conducted some experiments with amorphous SiO_2 and two kinds of silicon-rich industry wastes in greenhouse and field experiments. The silicon status, change of additional silicates and mineral neoformation were controlled by of element analyzing, x-ray, IR-spectroscopies and electronic microscopy.

The application of high active amorphous silicates had great influence on soil mineral phosphates (Ca-, Al-, Fe-). Our investigations showed possibility of the reaction of replacement Si on P in soil.

Conclusions:

1. The great amount of Si was involved by live organisms, essentially by plants.
2. The intensive agriculture pressure caused to negative changes of mineral equilibrium in soil.
3. The silica metal industry wastes can be used for restore and preserve of mineral equilibrium in cooper soils.

BARIUM-FREE BURBANKITE FROM POÇOS DE CALDAS, MINAS GERAIS, BRAZIL.

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Barium-free burbankite - $(\text{Na,Ca})_3(\text{Sr,Ce})_3(\text{CO}_3)_5$, hexagonal - occurs as a latest interstitial filling mineral in the nepheline sienite from Pedreira da Prefeitura ("City Hall Quarry"), Poços de Caldas, Minas Gerais, Brazil. Associated minerals in the fracture are calcite, fluorite, natrolite, analcite, pyrite, manganian ilmenite, strontianite, ankerite, kutnahorite, gaidonnayite and an unidentified chlorite-like mineral (cf. also Ulbrich & Ulbrich, 1992). Barium-free burbankite forms colorless to yellowish euhedral, individual or radial aggregates of prismatic to acicular crystals up to 10 mm. The mineral is optically uniaxial negative with $\omega = 1.620$ and $\epsilon = 1.600$. X-ray powder-diffraction data for the Brazilian sample are virtually identical to those cited in the literature. EDS analysis showed the presence of Sr, Na, Ca and Ce. Poços de Caldas burbankite differs from the samples from other occurrences (chemical analyses of burbankite from several localities quoted by Fitzpatrick & Pabst, 1977) by the absence of Ba. Barium-free burbankite was synthesized by Chen & Chao (1974).

References:

- Chen, T.T. & Chao, G.Y. (1974). *Can. Mineral.*, 12, 342-345.
Fitzpatrick, J. & Pabst, A. (1977). *Am. Mineral.* 62, 158-163.
Ulbrich, H.H.G.J. & Ulbrich, M.N.C. (1992). *Roteiro de Excursão*, v.5, 370. Congr. Bras. Geol.

MD SIMULATION OF CRYSTALS AND MELTS IN THE SYSTEM $\text{CaO-MgO-Al}_2\text{O}_3\text{-SiO}_2$

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Transferable interatomic potentials have been developed for use in computer simulations of both crystals and melts in the $\text{CaO-MgO-Al}_2\text{O}_3\text{-SiO}_2$ system. The potentials are composed of pairwise additive Coulomb, van der Waals and repulsive interactions. The net charges, q_i s, on the Ca, Mg, Al, Si, and O

ions are constrained as $q(\text{Ca}) = q(\text{Mg}) = \frac{2}{3}q(\text{Al}) = \frac{1}{2}q(\text{Si}) = -q(\text{O})$, in order to preserve the requirement of transferability between materials with different composition. Necessary energy parameters were obtained and tested using both the static WMIN and dynamic MD calculations for crystals in the system $\text{CaO-MgO-Al}_2\text{O}_3\text{-SiO}_2$.

The crystals studied here have a wide variety of structural topologies; including oxides (periclase, lime, corundum, and spinel), nesosilicates (olivines, garnets, and sillimanite), inosilicates (pyroxenes), and tectosilicates (cristobalite and quartz). Some high pressure phases, such as coesite, stishovite, wadsleyite, ringwoodite, MgSiO_3 ilmenite and perovskite, CaSiO_3 perovskite, are also included.

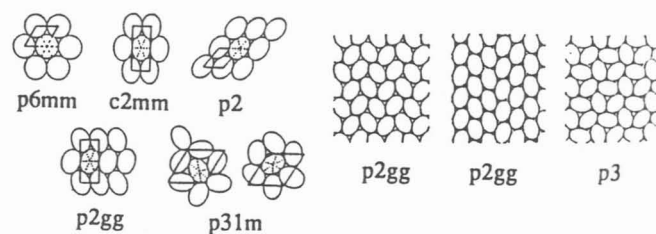
In spite of the simplicity of the potentials and the diversity of the structural types, our MD simulations are quite satisfactory in reproducing accurately the observed structures of these crystals, including the symmetries of the crystal lattices, the unit-cell parameters, the coordination numbers of the cations, and the Ca-O, Mg-O, Al-O and Si-O bond distances. The MD simulated bulk moduli of these minerals are also found to agree well with the measured values.

The MD calculations are further successfully used to reproduce reasonably well the measured (or estimated) densities of various melts in the system $\text{CaO-MgO-Al}_2\text{O}_3\text{-SiO}_2$, and their temperature and pressure dependence.

CLOSE PACKING OF IDENTICAL ELLIPSES

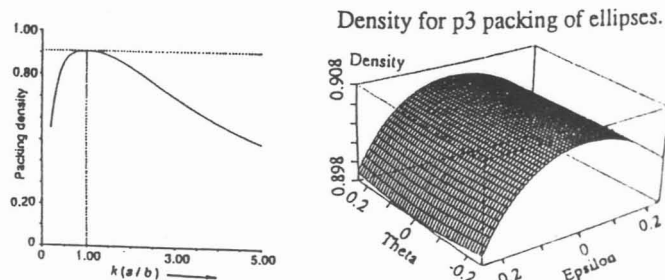
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In contrast with the closest packing of circles, with plane group p6mm, periodic close packings of ellipses with 6 contacting neighbours do not always have the maximum density $\rho = \pi/2\sqrt{3}$. Nowacki(1948) indicated five different densest packings of ellipses in four plane groups: p2, c2mm, p2gg and p31m, in 54 types of periodic patterns of ellipses. In all of these five packings, every ellipse is in contact with 6 neighbour ellipses. These packings could be considered to be the densest among the possible forms of ellipse packing.



Close packings of circles and ellipses. Nowacki(1948)

Close packing of ellipses. Grünbaum & Shephard(1987)



Density for p31m packing of ellipses. Tanemura & Matsumoto(1992)