21. STRUCTURAL RESULTS FROM METHODS OTHER THAN DIFFRACTION

21.1—1 STUDYING REAL STRUCTURE OF CRYSTALS BY DIELECTRIC SPECTROSCOPY.


Data on real structure of crystals obtained by universally accepted techniques (EPR, optical spectroscopy, combinational dissipation etc) may be far more numerous and complex if dielectric spectroscopy is used as a further-aid. It is especially important when point defects of the studied crystals are non paramagnetic, optically inactive though electrically active in non-excited state.

Quartz is a good example of these crystals. Electrically active point defects in quartz are known to be alkali metal ions that dominate there as the type.

We have compared experimental temperature/frequency dependencies $\varepsilon'$ at temperatures of 300-800 K with Debye theoretical curve and presented Cole-Cole and Scalis diagrams. As a result we state a presence of a broad energy spectrum of impurity alkali ions. Energy distribution is not Gaussian, the observed asymmetry of normalised $\varepsilon'(\omega)$ function proving it. The distribution parameter of relaxation time ($\alpha$) increases with crystallisation temperature and with lower rates of growth.

We have postulated presence of $\text{H}_2\text{O}$ molecules in structure voids of cancrinite crystals using energy parameters of relaxation polarisation in a temperature range of 350-500 K. We have calculated the $\alpha$ value to change from 0.05 to 0.40 at temperatures of 350-500 K. This change may result from multiple structure positions of $\text{H}_2\text{O}$ molecules and their reorientations at various temperatures (Kolodiev et al., Sintex miner. i exper. issled., Moskva (1984) 21).

Dielectric spectroscopy approach to non-relaxation maxima $\varepsilon'(T)$ should be very careful. In interpreting of the experimental results special attention should be paid to reversibility of the observed changes of the dielectric characteristics and to their correlation to other physical properties.

For example, we can state that the non-relaxation maximum $\varepsilon'(T)$ in region of 650-800 K in cancrinite is not reproducible at repeated heating. This fact may result from irreversible changes of cancrinite structure further corroborated by substantial weakening of its piezo effect after heating to 800 K.

Similar maxima of $\varepsilon'(T)$ obtained during heating of fluorphlogopite (up to 900 K) are reproducible, though after certain intervals of time. This is a case of reversible processes with great relaxation time of the crystal to the initial state. General phenomenology may describe this process as a recombination of defects that determine dielectric losses with acceptor centers thermally activated in this temperature range to form metastable pairs (or complexes) that dissociate later on (Kolodiev et al., Vees. neutchn. konfer. "Physikal. dielektriev". Sektional "Protesty elektroenergias". Thesis. dokladov, Baku (1982) 63).