the Mahabaleshwar area of Maharashtra state, India. The feldspar phenocrysts contain different types of melt inclusions. These melt inclusions significantly show variation in melting temperature. Presence of different types of melt inclusions along crystal boundaries indicated the change in composition and this may be the function of temperature. Different types of melt inclusions found in plagioclase phenocrysts are amorphous and crystalline (monophase, biphase and multiphase).Variation in the commodity of these melt inclusions, itself reveals the immiscibility as well as the degassing phenomena of magma. An attempt has been made to correlate the melt inclusion geothermometry with the evolution pattern of magma/melt that of calcic-plagioclase phenocrysts present in a deccan basalts. Petrographic results were confirmed by the XRD and Cathodoluminescence studies. Heating stage experiment was carried out to find out the formation temperatures/melting temperatures of melt inclusions.

Keywords: geothermometry, melt inclusion, crystallography

P10.02.04

Calculation of graphs representing crystal structures

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Some crystal structures can be described by certain graphs (Chung & Hahn, Acta Cryst. A31 (1975) S.J. Chung, Hahn & Klee, Acta Cryst. A40 (1984) 42-50). In this method, each periodic infinite net can be expressed by a labelled directed finite graph which is called also labelled quotient graph. Each point and each line in the quotient graph corresponds to a set of equivalent vertices and edges in the three periodic net. Quotient graphs and spanning trees can obtained with given numbers of vertices and edges in this calculation. We use the determinant and trace of the matrix representing the quotient graph for the criteria of isomorphism of quotient graph. Special algorithm is applied to this program because the isomorphism of quotient graphs seriously delays the computation time with increase of the number of vertices and edges. The labelling to the quotient graphs can be applied. The structure of the network also can be obtained from the labelled graphs with least square fitting. A computation method for the enumeration of three periodic regular nets with a given number of vertices and edges will be discussed in detail.

Keywords: graph, network, crystal structure

P10.02.05

Hybrid twins in minerals

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Twins in which the lattice nodes (quasi) restored by the twin operation belong to more than one sublattice are termed *hybrid twins* [1]. The fraction of (quasi) restored nodes takes into account all these sublattices and an *effective twin index n_E* is defined. In Friedelian twins (twin index not higher than 6), the hybrid character shows that the choice of the sublattice is not unique. In non-Friedelian twins, n_E allows a rationalization of these twins within the framework of the classical reticular theory [2]. A survey of twins in minerals has shown that a number of them should be reinterpreted as hybrid twins. For high-symmetry twins (cubic and uniaxial minerals), this is normally the case for twin elements of relatively high indices. E.g., (031) twin in cassiterite (four sublattices, $n_E = 3.8$), (311) twin in nickeline (three sublattices, $n_E = 6.3$), (203) twin in maucherite (three sublattices, $n_E = 5.83$, (241) twin in diaphorite (two sublattices, $n_E = 4.0$), and [313] twin in staurolite (two sublattices, $n_E = 6.0$). For lower symmetry minerals, even low-index twin elements may correspond to a non-Friedelian twin that is better interpreted as hybrid twins. E.g., (110) twin in becquerelite (three sublattices, $n_E = 3.0$), (110) twin in geocronite (three sublattices, $n_E = 3.0$), and (211) twin in cryolite (three sublattices, $n_E = 3.7$). Examples of Friedelian twin that can be interpreted as hybrid twins have also been found; e.g., (011) twin in anhydrite: here one sublattice corresponds to index 4 and obliquity 0.7º, another sublattice to index 3 and obliquity 3.1º. If both sublattices are taken into account, one obtains $n_E = 2.0$.

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Keywords: twinning, hybrid twins, effective twin index

P10.02.06

Atomic displacements of tetrahedral cations in garnets

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We had reported that in most of reported garnets, the root mean-square displacements (RMSD) of tetrahedral (*Z*) cations are the smallest in the directions of adjacent dodecahedral (*X*) cations (direction 1), parallel to a crystal axis, because of strong *X*-*Z* repulsions and the largest in the directions of the remaining two crystal axes (direction 2). However, we recently found that RMSD of *Z* cation in Pb vanadate garnets ($NaPb_2M_2V_3O_{12}$; *M* is divalent cations) is the largest in the direction 1, in which adjacent *X* cations exist, and the smallest in the direction 2, in which no adjacent atoms exist, in contradiction to the above general tendency. In the present study, to examine whether this peculiar feature in Pb vanadate garnets is due to the positional disorder of *Z* cation toward the direction 1 caused by lone pair electrons of Pb^{2+} in *X* site, we perform the structure refinements of $NaSr_2Mg_2V_3O_{12}$, having *X* cation (Sr^{2+}) without lone pair electrons and expected to possess *X*-*Z* repulsion comparable to those in Pb vanadate garnets, at 298 K and $NaPb_2Mg_2V_3O_{12}$ in the range of 83-298 K. Moreover, the crystal structures of uninvestigated Ca vanadate garnets ($NaCa_2Co_2V_3O_{12}$, $NaCa_2Ni_2V_3O_{12}$) are refined at 298 K. $RMSD_1/RMSD_2$ ratios of *Z* cations (V^{5+}) in $NaCa_2Co_2V_3O_{12}$ and $NaCa_2Ni_2V_3O_{12}$ are below 1.0 according to the general tendency, whereas that in $NaSr_2Mg_2V_3O_{12}$ is much larger than 1.0 as in Pb vanadate garnets, where $RMSD_1$ and $RMSD_2$ are RMSD's in the directions 1 and 2, respectively. The U_{eq} value in *Z* cation of $NaPb_2Mg_2V_3O_{12}$ can be extrapolated to 0 at 0 K, and no separation of electron density peak on *Z* site can be observed on Fourier map. These show that the peculiar atomic displacement behavior of *Z* cation in Pb vanadate garnets cannot be due to its positional disorder.

Keywords: crystal chemistry, thermal vibration, single-crystal