The Bond Valence Model and Point Defects in Langasite Family

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Crystals of langasite structure ($La_3Ga_5SiO_{14}$ - $La_3Ga(1)Ga_3(2)(GaSi)(3)O_{14}$) belong to the sp.gr. P321 and have four kinds of cation sites. The La, Ga(1), Ga(2) and (GaSi)(3) ions are located on a decahedral, octahedral, tetrahedral and trigonal-pyramidal sites, respectively.

In this work we demonstrate an analysis of the structure refinements of the langasite family compounds $La_3Ga_4(Ga_xSi_{2-x})O_{14}$, $La_3Ga_4[Ga(Si,Ge)]O_{14}$, $La_3Ga_{5.5}M_{0.5}O_{14}$ c M=Ta, Nb with the bond valence models. The calculation of bond valence (s_{ij}) for cation sites was made by the two methods:

- method of Brese and O'Keeffe: $s_{ij}=\exp[(R_{ij} - d_{ij})/b]$;
- method of Brown and Wu: $s_{ij}=(R_i/d_{ij})^{-N}$

The calculation of s_{ij} valus for cation and anion sites was fulfiled by Pyatenko method: $s_{ij} = k_i/d_{ij}^{n}$; $k_i=\upsilon_{kj}/\Sigma d_{ij}^{-n}$ (d_{ij} –cation-anion distance).

With these results, it is possible to confirm the occupancy of the (GaSi)(3) sites by some cations and their correlation, to suppose a presence of cation vacancies in La and Ga(1) sites, to prove a distribution of the Ta and Nb ions into two sites (Ga(1) and (GaSi)(3)) and one site (Ga(1)), respectively.

Keywords: langasite, point defects, bond valence method