Crystal-field analysis for RE^{3+} ions in laser materials: III. Energy levels for Nd^{3+} and Er^{3+} ions in $LaAlO_3$, $YAlO_3$ and $LaGaO_3$ single crystals - combined approach to low symmetry crystal field parameters.

Autorzy

Mirosław Karbowiak

Paweł Gnutek

Czesław Rudowicz

Rok wydania

2012

Czasopismo

Chemical Physics

Numer woluminu

400

Strony

29-38

DOI

10.1016/j.chemphys.2012.01.021

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Crystal field (CF) analysis of energy levels for Nd^{3+} and Er^{3+} ions in $LaAlO_3$, $YAlO_3$, and $LaGaO_3$ single crystals is presented. It is shown that a combined approach comprising the ascent/descent in symmetry (ADS) method combined with superposition model (SPM) analysis can be successfully used for analysis of low-symmetry systems. The present ADS/SPM approach is less labor and time consuming as compared, e.g., with Monte-Carlo method and it also allows maintaining the relationship between the crystallographic axis system and the nominal axis systems of fitted CFP sets. For orthogallates and orthoaluminates the actual C_s symmetry, resulting from distortion of perovskite structure, may be successfully approximated for both systems by the ADS chain $C_{4v} \leftrightarrow C_3$ $(D_3) \leftrightarrow C_s$ or C_3 $(D_3) \leftrightarrow C_s$ symmetry. The possibility of using of approximated symmetries for orthogallates or orthoaluminates can be useful for interpretation of energy levels for this family of compounds of technological importance, particularly in the case when the number of available experimental energy levels is insufficient for full C_s parameterization. The novel aspect of the combined ADS/SPM approach is that possible higher symmetry approximations employing also the axis systems oriented differently than for the actual symmetry are searched for, taking advantages of the transformation properties of CF parameters sets.

Słowa kluczowe

Optical spectroscopy, Crystal (ligand) field parameters, Monoclinic site symmetry, Low-symmetry, Nd3+ ions, Er3+ ions, LaAlO3, YAlO3, LaGaO3

Adres publiczny

https://doi.org/10.1016/j.chemphys.2012.01.021