Crystallochemical affinity and optical functions of $ZrGa_2$ and $ZrGa_3$ compounds

Abstract

The influence of crystallochemical affinity for crystals $ZrGa_2$ and $ZrGa_3$ on the optical properties was studied. We have calculated dispersion of optical constants ε2average(ω). We have established that application of different exchange correlation potentials XC has no significant effect on the optical constant dispersion. Moreover, use of LDA, GGA and EVGGA has an insignificant effect on the corresponding optical features. The crystallochemical transformation between the two titled compounds leads to a spectral shift of the whole ε2average(ω) structure: for $ZrGa_3$ it leads to higher energy shift with respect to $ZrGa_2$. Moreover, one can see that the first spectral peak of ε2average(ω) for $ZrGa_2$ which situated at around 0.5 eV becomes very small for $ZrGa_3$ but still situated in the same location. The first right hand side hump in ε2average(ω) - $ZrGa_2$ which is located at around 1.5 eV becomes pronounced and situated at around 2.2 eV in ε2average(ω) - $ZrGa_3$. For more complete information we have calculated dispersions of the electronic loss function, reflectivity and the optical conductivity.